



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 08:53 AM UTC

PDB ID : 4V7T / pdb_00004v7t
Title : Crystal structure of the E. coli ribosome bound to chloramphenicol.
Authors : Dunkle, J.A.; Xiong, L.; Mankin, A.S.; Cate, J.H.D.
Deposited on : 2010-08-14
Resolution : 3.19 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

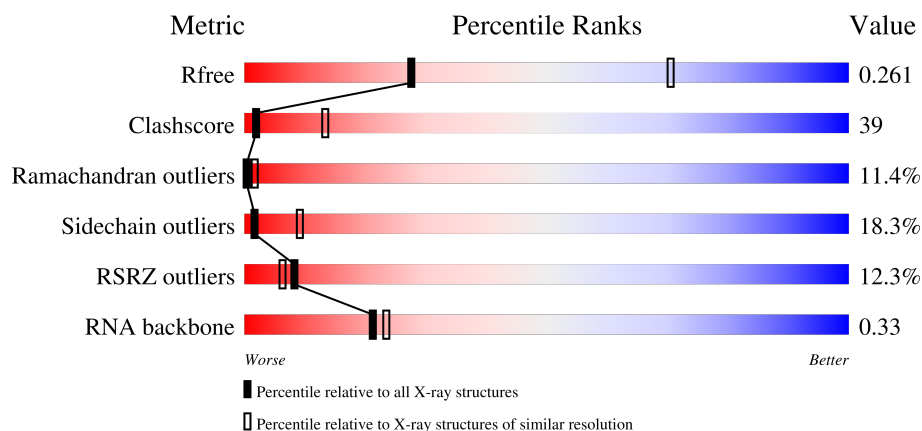
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1533	24% 45% 20% 11%
2	AB	218	7% 22% 55% 19% .
2	CB	218	14% 29% 55% 14% .
3	AC	206	3% 34% 52% 11% .

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Mol	Chain	Length	Quality of chain
3	CC	206	
4	AD	205	
4	CD	205	
5	AE	150	
5	CE	150	
6	AF	100	
6	CF	100	
7	AG	151	
8	AH	129	
8	CH	129	
9	AI	127	
9	CI	127	
10	AJ	98	
10	CJ	98	
11	AK	117	
11	CK	117	
12	AL	123	
12	CL	123	
13	AM	114	
14	AN	100	
14	CN	100	
15	AO	88	
15	CO	88	
16	AP	82	
17	AQ	80	

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Mol	Chain	Length	Quality of chain
17	CQ	80	
18	AR	55	
18	CR	55	
19	AS	79	
19	CS	79	
20	AT	85	
20	CT	85	
21	AU	51	
21	CU	51	
22	BA	2903	
23	BB	118	
24	BC	271	
24	DC	271	
25	BD	209	
25	DD	209	
26	BE	201	
26	DE	201	
27	BF	177	
28	BG	176	
28	DG	176	
29	BH	149	
29	DH	149	
30	BI	141	
30	DI	141	
31	BJ	142	

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Mol	Chain	Length	Quality of chain
31	DJ	142	
32	BK	122	
32	DK	122	
33	BL	143	
33	DL	143	
34	BM	136	
34	DM	136	
35	BN	120	
35	DN	120	
36	BO	116	
36	DO	116	
37	BP	114	
37	DP	114	
38	BQ	117	
38	DQ	117	
39	BR	103	
39	DR	103	
40	BS	110	
40	DS	110	
41	BT	93	
41	DT	93	
42	BU	102	
42	DU	102	
43	BV	94	
43	DV	94	

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Mol	Chain	Length	Quality of chain
44	BW	79	
44	DW	79	
45	BX	77	
45	DX	77	
46	BY	63	
46	DY	63	
47	BZ	58	
47	DZ	58	
48	B0	56	
48	D0	56	
49	B1	50	
49	D1	50	
50	B2	46	
50	D2	46	
51	B3	64	
51	D3	64	
52	B4	38	
52	D4	38	
53	CA	1530	
54	CG	150	
55	CM	113	
56	CP	80	
57	DA	2904	
58	DB	117	
59	DF	178	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	DA	3062	-	-	-	X
60	MG	DA	3073	-	-	-	X
60	MG	DA	3124	-	-	-	X

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 284499 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	218	Total	C	N	O	S	0	0	0
			1705	1081	305	312	7			
2	CB	218	Total	C	N	O	S	0	0	0
			1705	1081	305	312	7			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			
3	CC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			
4	CD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	CE	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			818	515	148	149	6			
6	CF	100	Total	C	N	O	S	0	0	0
			818	515	148	149	6			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
8	CH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
9	CI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			
10	CJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			
11	CK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			
12	CL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
14	CN	95	Total	C	N	O	S	0	0	0
			769	480	159	127	3			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
15	CO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			
17	CQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AR	55	Total	C	N	O	S	0	0	0
			456	288	86	82				
18	CR	55	Total	C	N	O	S	0	0	0
			456	288	86	82				

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			
19	CS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			
20	CT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			
21	CU	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			

- Molecule 23 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			

- Molecule 24 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			
24	DC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			
25	DD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

- Molecule 26 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			
26	DE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

- Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BF	177	Total	C	N	O	S	0	0	0
			1411	899	249	257	6			

- Molecule 28 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			
28	DG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			
29	DH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			

- Molecule 30 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			
30	DI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

- Molecule 31 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
31	DJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BK	122	Total	C	N	O	S	0	0	0
			939	587	180	166	6			
32	DK	122	Total	C	N	O	S	0	0	0
			939	587	180	166	6			

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			
33	DL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

- Molecule 34 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			
34	DM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BN	120	Total	C	N	O	S	0	0	0
			961	593	196	167	5			
35	DN	120	Total	C	N	O	S	0	0	0
			961	593	196	167	5			

- Molecule 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	BO	116	Total	C	N	O	0	0	0
			892	552	178	162			
36	DO	116	Total	C	N	O	0	0	0
			892	552	178	162			

- Molecule 37 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
37	DP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 38 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
38	BQ	117	Total	C	N	O	0	0	0
			947	604	192	151			
38	DQ	117	Total	C	N	O	0	0	0
			947	604	192	151			

- Molecule 39 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	DR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 40 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			
40	DS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BT	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			
41	DT	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BU	102	Total	C	N	O		0	0	0
			780	492	146	142				
42	DU	102	Total	C	N	O		0	0	0
			780	492	146	142				

- Molecule 43 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
43	DV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			
44	DW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			

- Molecule 45 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
45	DX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			
46	DY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

- Molecule 47 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
47	DZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
48	D0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	B1	50	Total	C	N	O	0	0	0
			410	263	75	72			
49	D1	50	Total	C	N	O	0	0	0
			410	263	75	72			

- Molecule 50 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
50	D2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
51	D3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
52	D4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 53 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	CA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			

- Molecule 54 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	CG	150	Total	C	N	O	S	0	0	0
			1175	730	226	215	4			

- Molecule 55 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	CM	113	Total	C	N	O	S	0	0	0
			877	541	177	156	3			

- Molecule 56 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	CP	80	Total	C	N	O	S	0	0	0
			639	400	126	112	1			

- Molecule 57 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	DA	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

- Molecule 58 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	DB	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

- Molecule 59 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	DF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

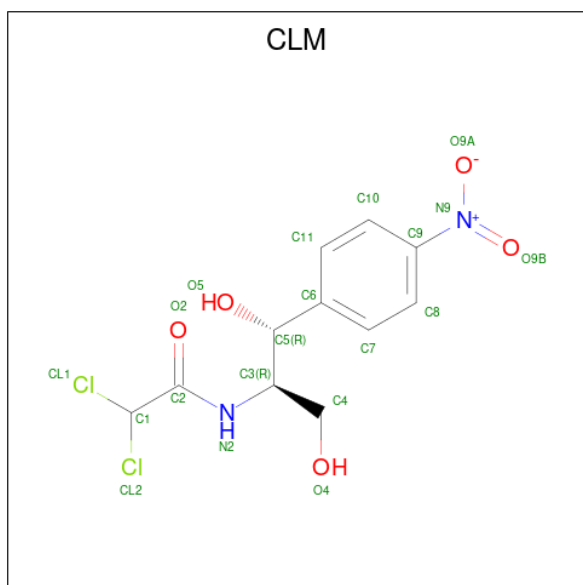
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AA	42	Total	Mg	0	0
			42	42		
60	AN	1	Total	Mg	0	0
			1	1		
60	BA	135	Total	Mg	0	0
			135	135		
60	BB	4	Total	Mg	0	0
			4	4		
60	BL	1	Total	Mg	0	0
			1	1		
60	CA	42	Total	Mg	0	0
			42	42		
60	DA	133	Total	Mg	0	0
			133	133		
60	DB	1	Total	Mg	0	0
			1	1		
60	DC	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	DE	1	Total	Mg	0	0
			1	1		
60	DJ	1	Total	Mg	0	0
			1	1		

- Molecule 61 is CHLORAMPHENICOL (CCD ID: CLM) (formula: $C_{11}H_{12}Cl_2N_2O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
61	BA	1	Total	C	Cl	N	O	0	0
			20	11	2	2	5		

- Molecule 62 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	B4	1	Total	Zn	0	0
			1	1		
62	D4	1	Total	Zn	0	0
			1	1		

- Molecule 63 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	AA	197	Total	O	0	0
			197	197		
63	AL	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	AN	6	Total 6	O 6	0	0
63	AT	2	Total 2	O 2	0	0
63	AU	1	Total 1	O 1	0	0
63	BA	608	Total 608	O 608	0	0
63	BB	19	Total 19	O 19	0	0
63	BC	8	Total 8	O 8	0	0
63	BD	2	Total 2	O 2	0	0
63	BE	1	Total 1	O 1	0	0
63	BL	4	Total 4	O 4	0	0
63	BN	2	Total 2	O 2	0	0
63	BQ	1	Total 1	O 1	0	0
63	BT	2	Total 2	O 2	0	0
63	BV	1	Total 1	O 1	0	0
63	B2	2	Total 2	O 2	0	0
63	B3	2	Total 2	O 2	0	0
63	B4	2	Total 2	O 2	0	0
63	CA	195	Total 195	O 195	0	0
63	CE	3	Total 3	O 3	0	0
63	CI	1	Total 1	O 1	0	0
63	CL	1	Total 1	O 1	0	0
63	CN	3	Total 3	O 3	0	0

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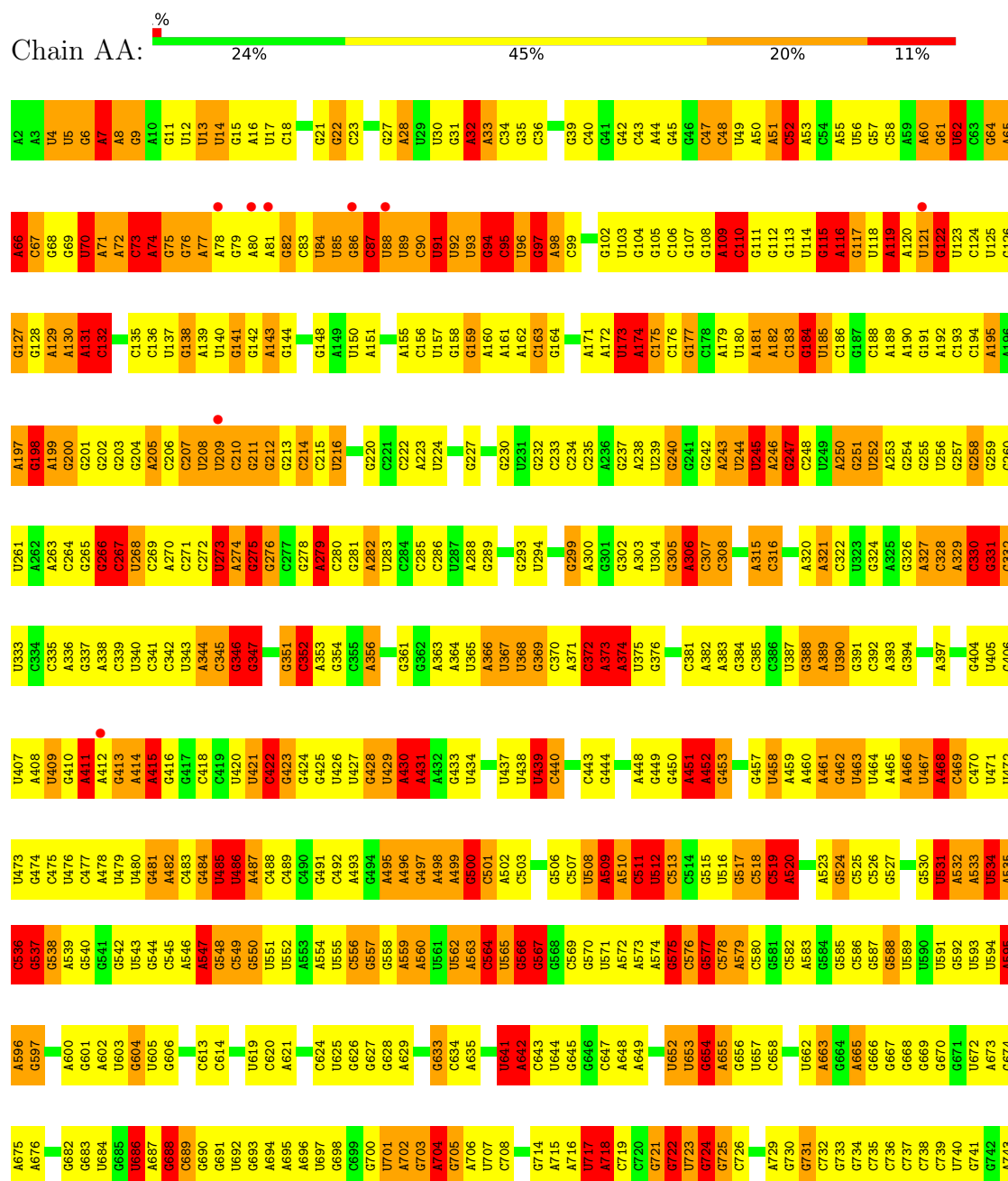
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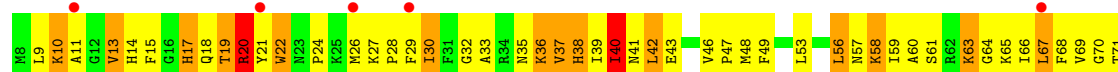
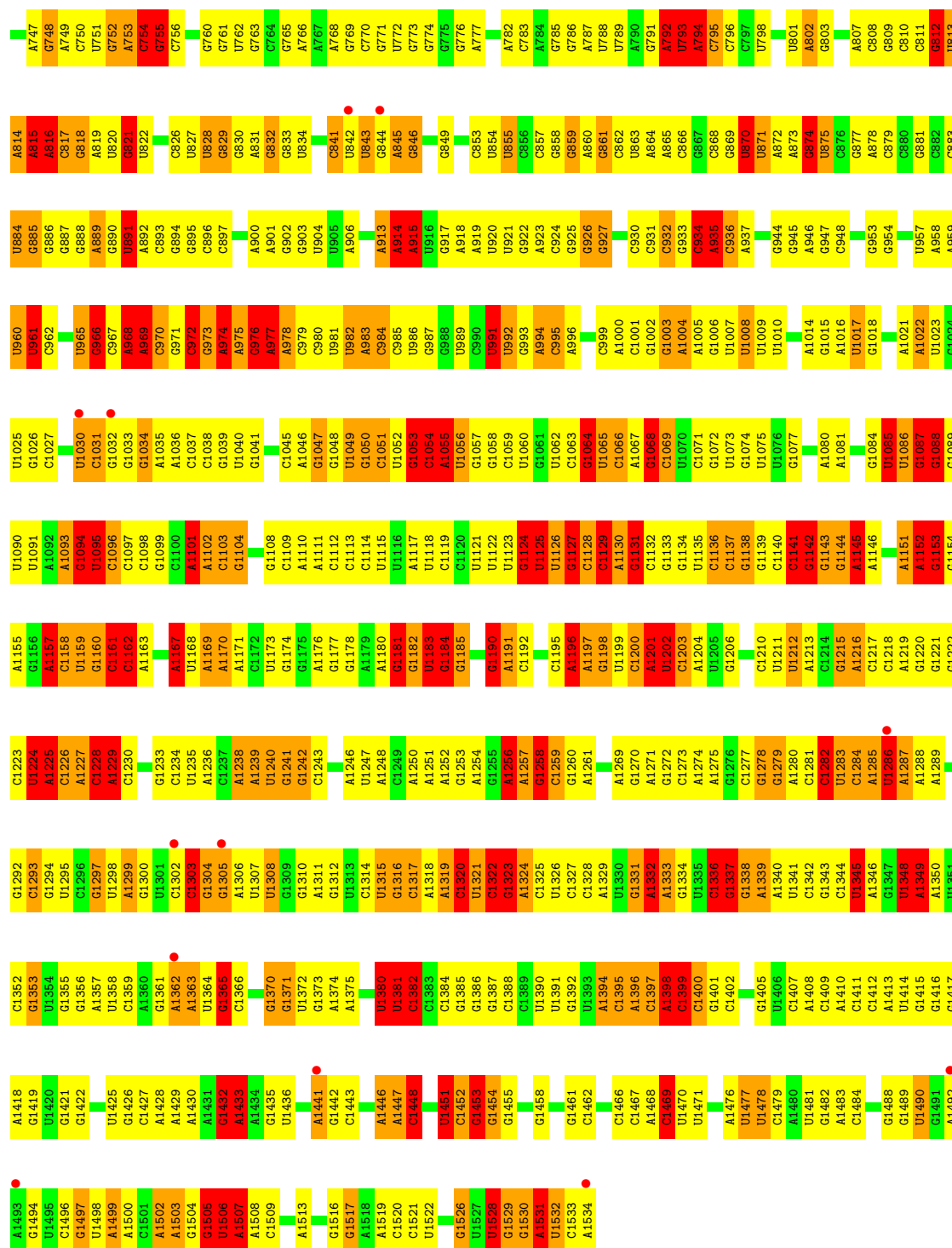
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	CT	2	Total O 2 2	0	0
63	CU	2	Total O 2 2	0	0
63	DA	603	Total O 603 603	0	0
63	DB	4	Total O 4 4	0	0
63	DC	10	Total O 10 10	0	0
63	DD	1	Total O 1 1	0	0
63	DE	3	Total O 3 3	0	0
63	DJ	4	Total O 4 4	0	0
63	DL	5	Total O 5 5	0	0
63	DN	2	Total O 2 2	0	0
63	DT	2	Total O 2 2	0	0
63	DU	2	Total O 2 2	0	0
63	DV	1	Total O 1 1	0	0
63	D2	1	Total O 1 1	0	0
63	D3	1	Total O 1 1	0	0
63	D4	4	Total O 4 4	0	0

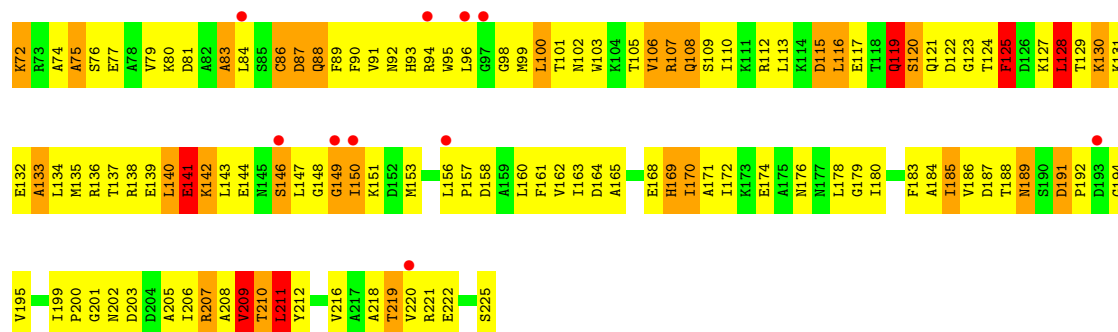
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

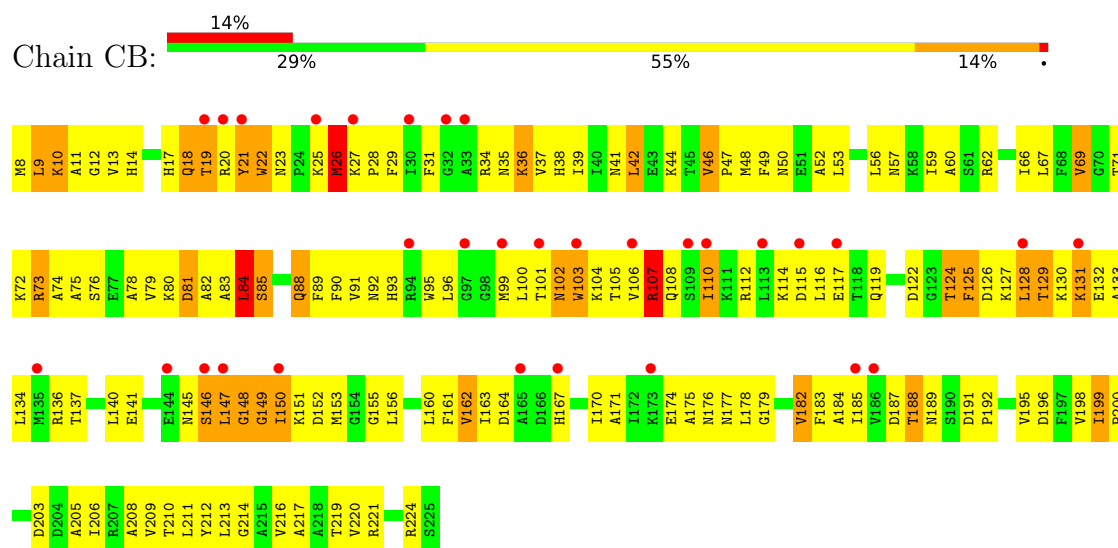
• Molecule 1: 16S rRNA



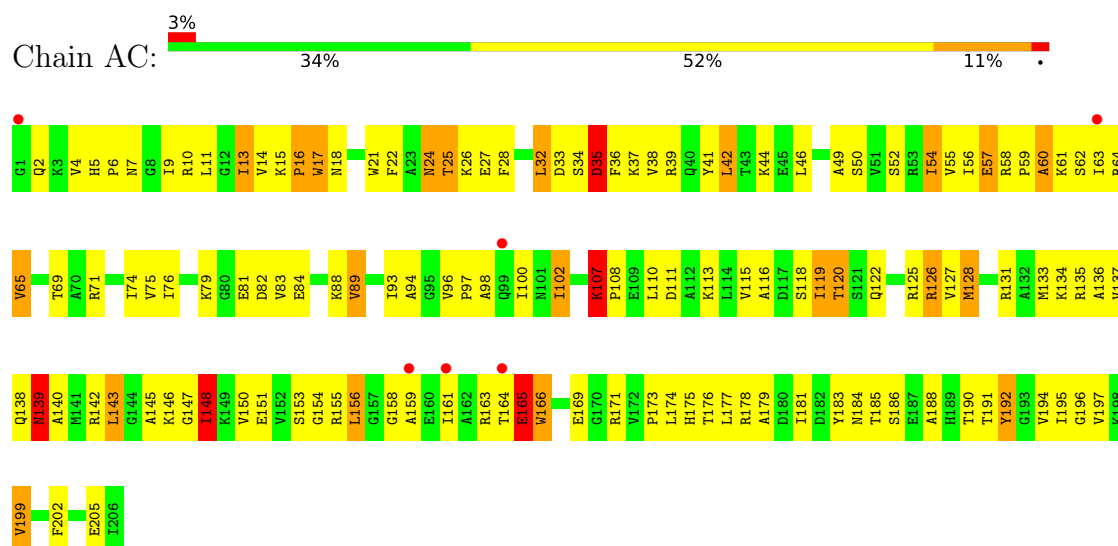




• Molecule 2: 30S ribosomal protein S2

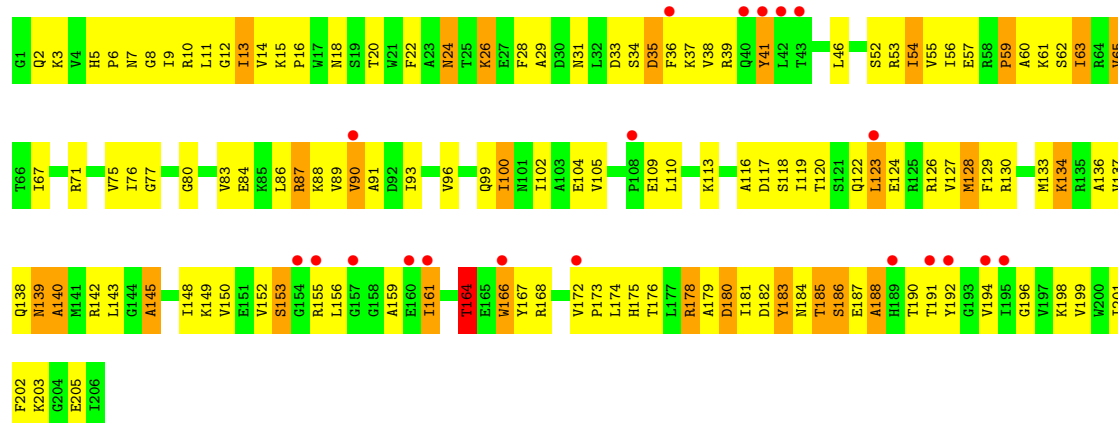


• Molecule 3: 30S ribosomal protein S3

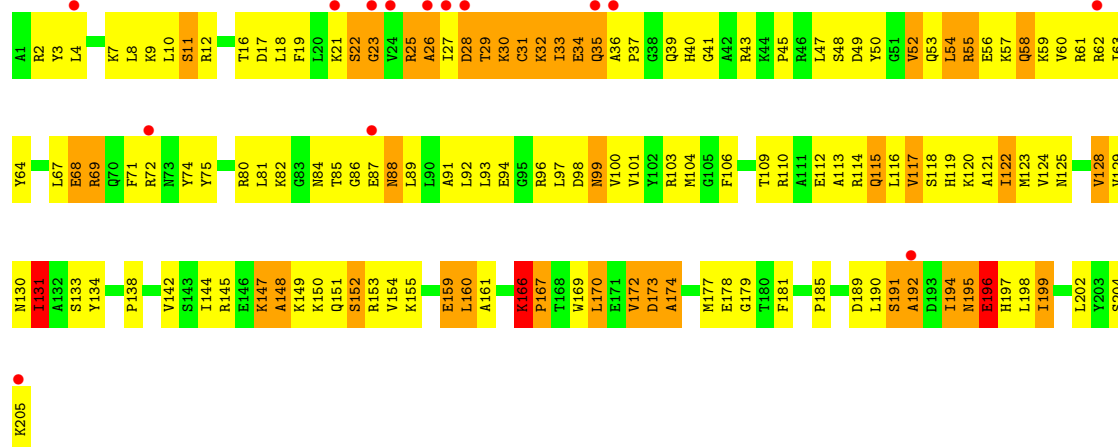


• Molecule 3: 30S ribosomal protein S3

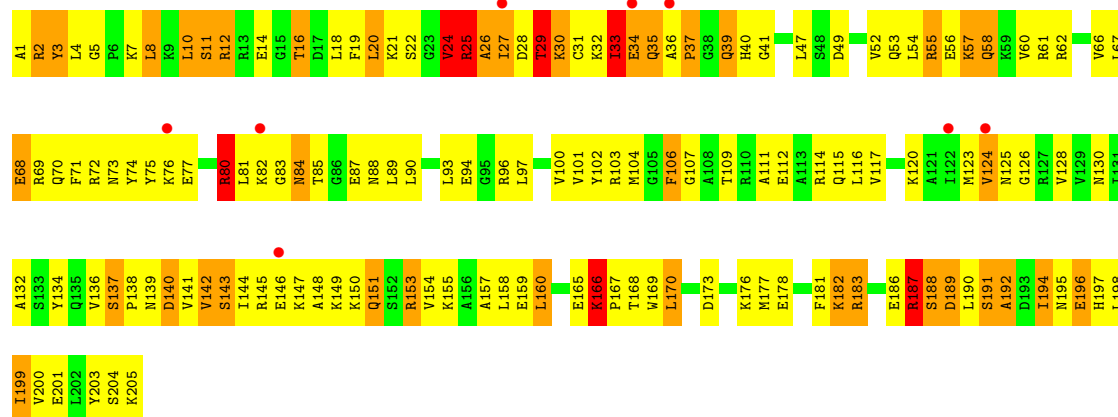




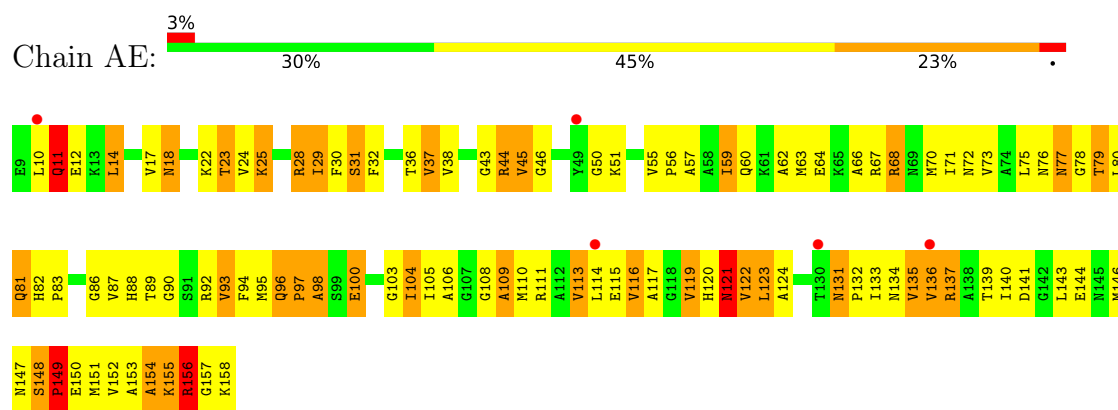
• Molecule 4: 30S ribosomal protein S4



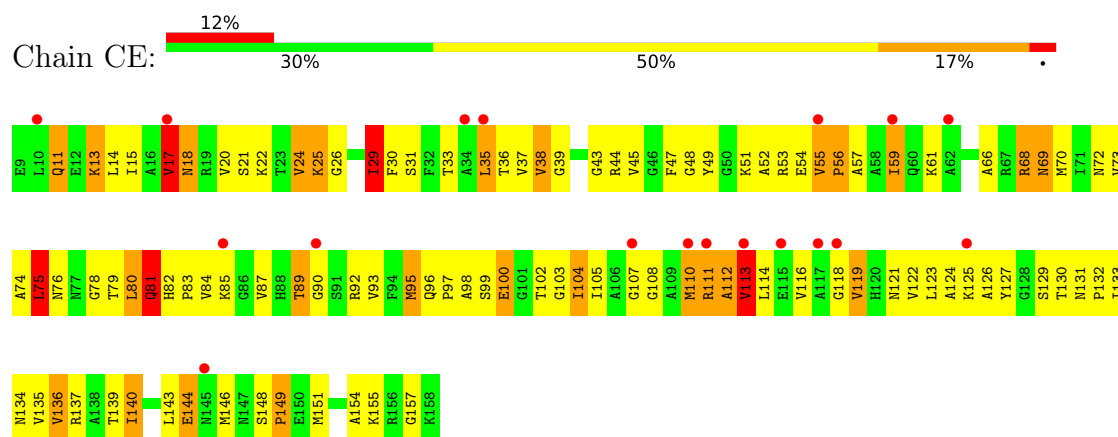
• Molecule 4: 30S ribosomal protein S4



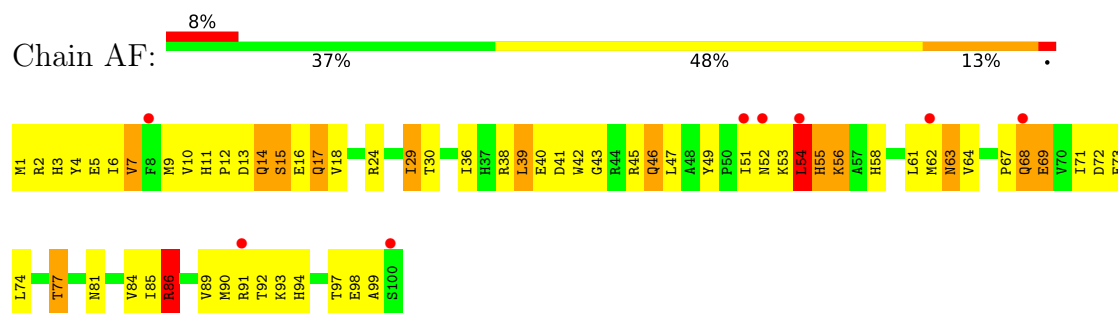
• Molecule 5: 30S ribosomal protein S5



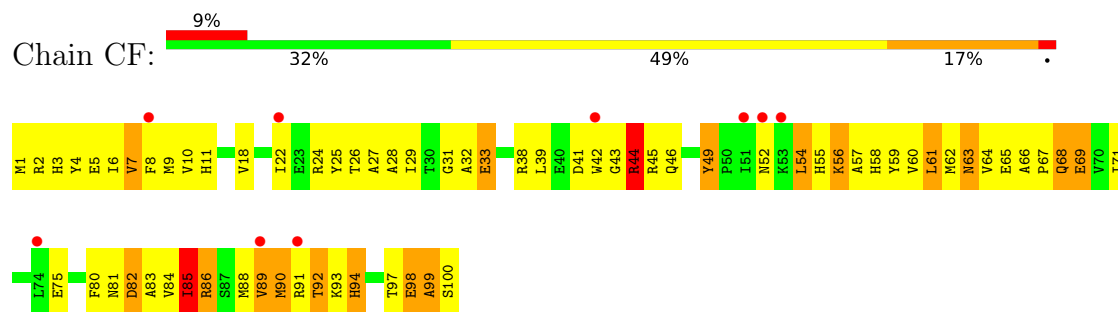
• Molecule 5: 30S ribosomal protein S5



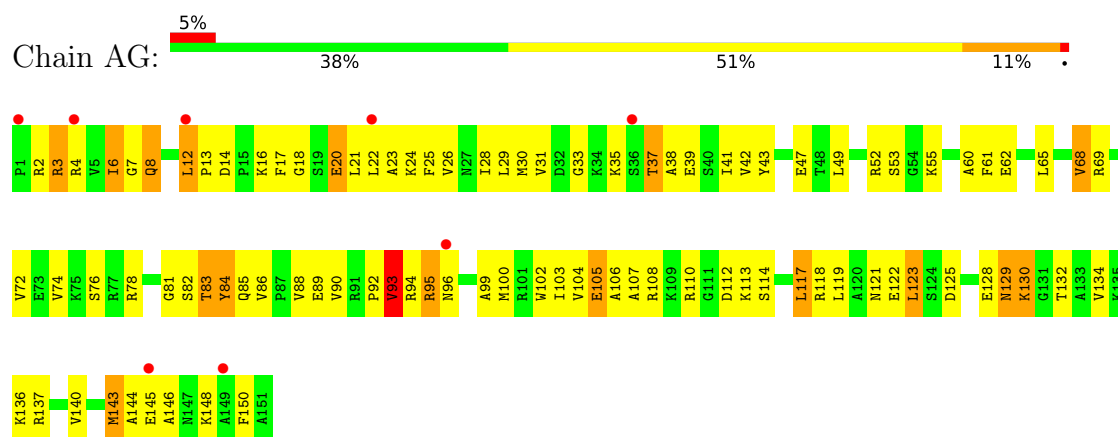
• Molecule 6: 30S ribosomal protein S6



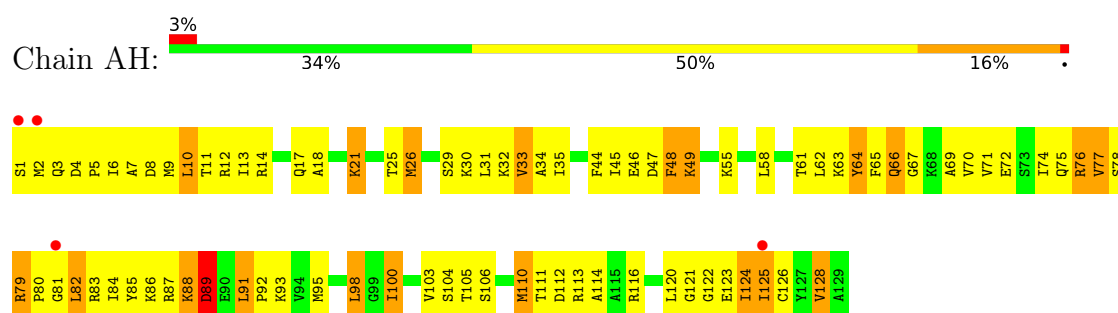
• Molecule 6: 30S ribosomal protein S6



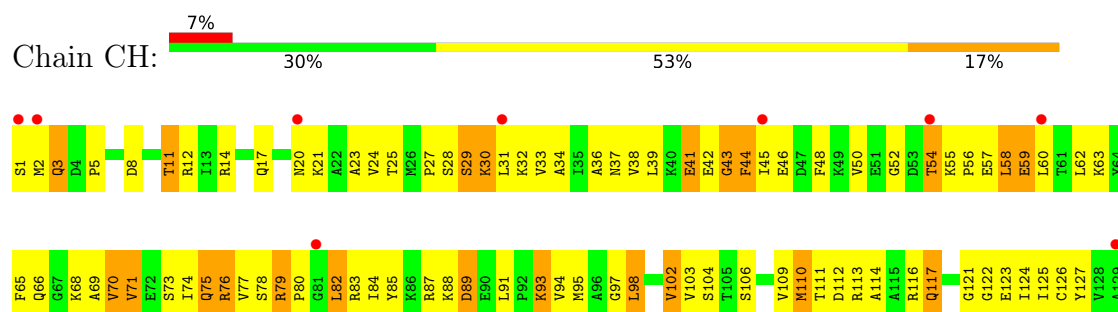
• Molecule 7: 30S ribosomal protein S7



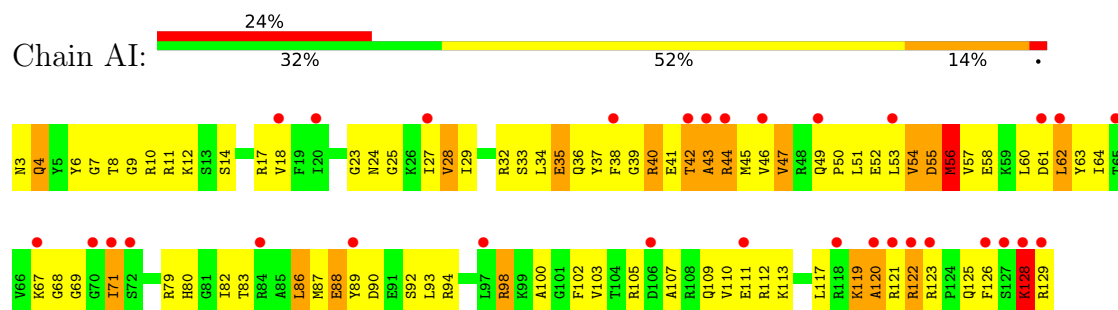
• Molecule 8: 30S ribosomal protein S8



• Molecule 8: 30S ribosomal protein S8

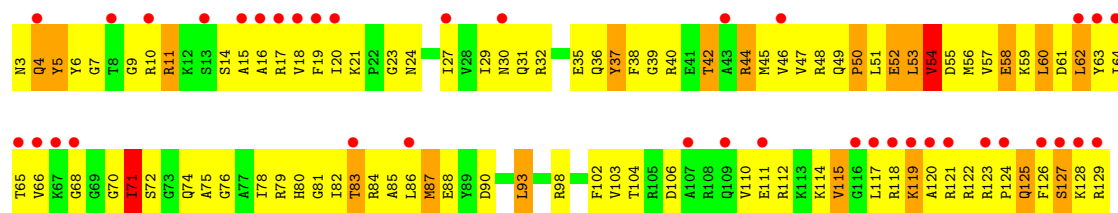


• Molecule 9: 30S ribosomal protein S9

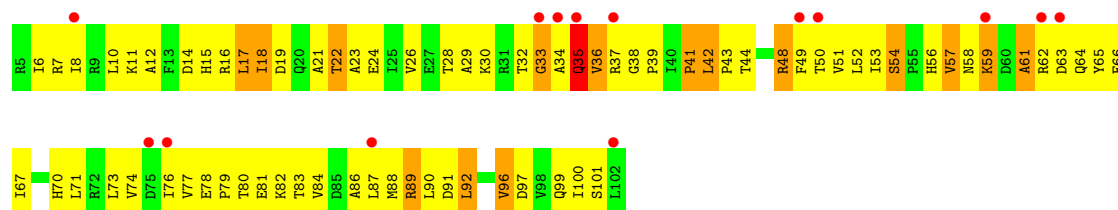


• Molecule 9: 30S ribosomal protein S9

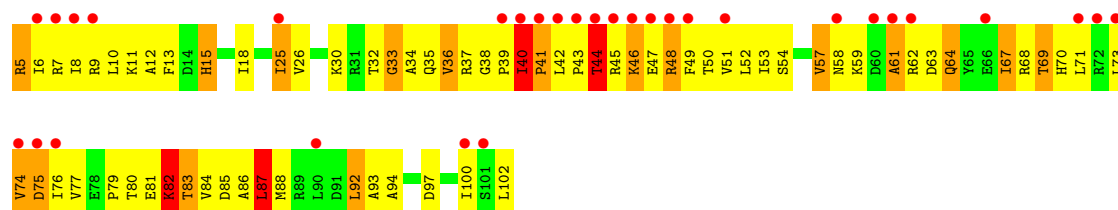




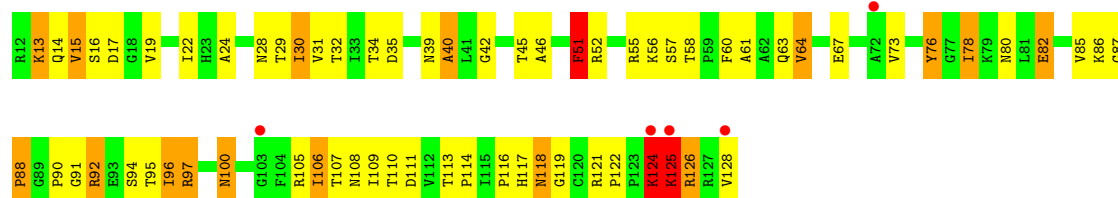
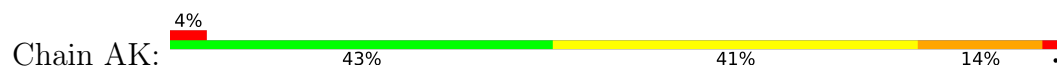
• Molecule 10: 30S ribosomal protein S10



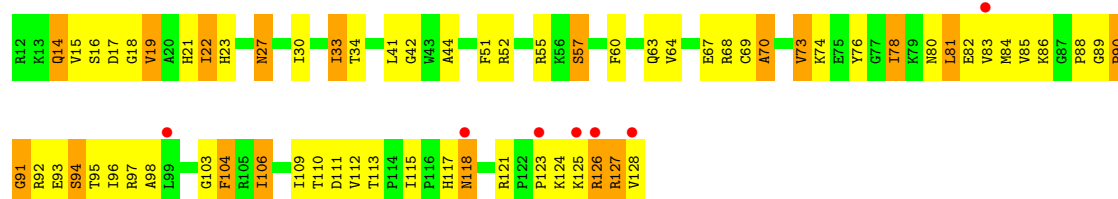
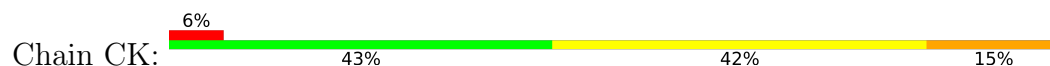
• Molecule 10: 30S ribosomal protein S10



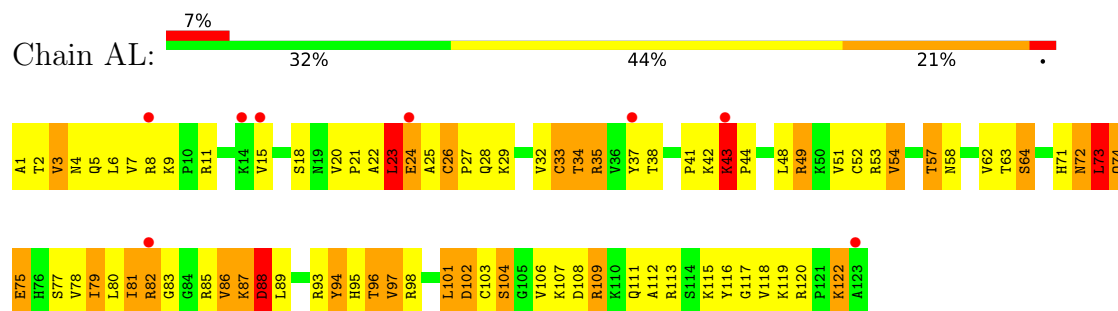
• Molecule 11: 30S ribosomal protein S11



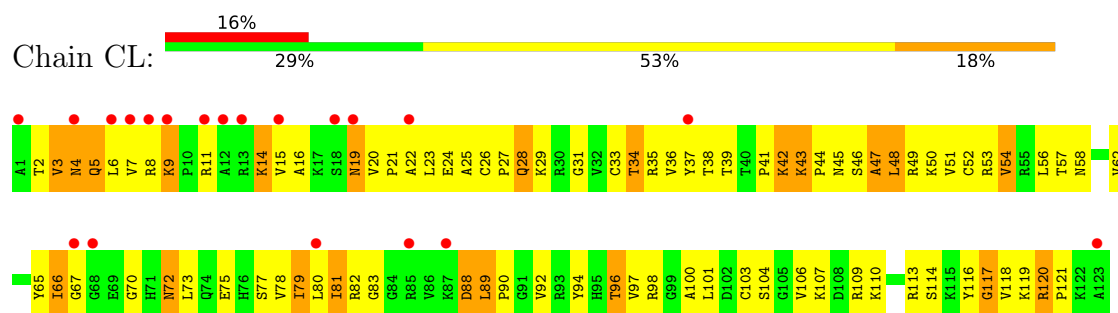
• Molecule 11: 30S ribosomal protein S11



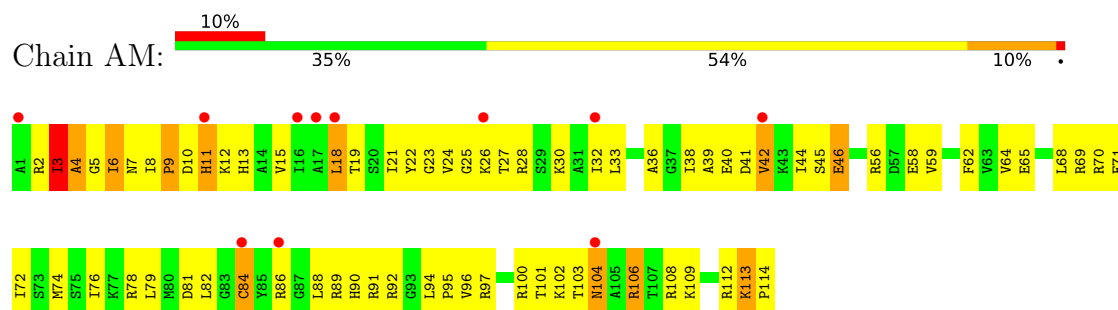
- Molecule 12: 30S ribosomal protein S12



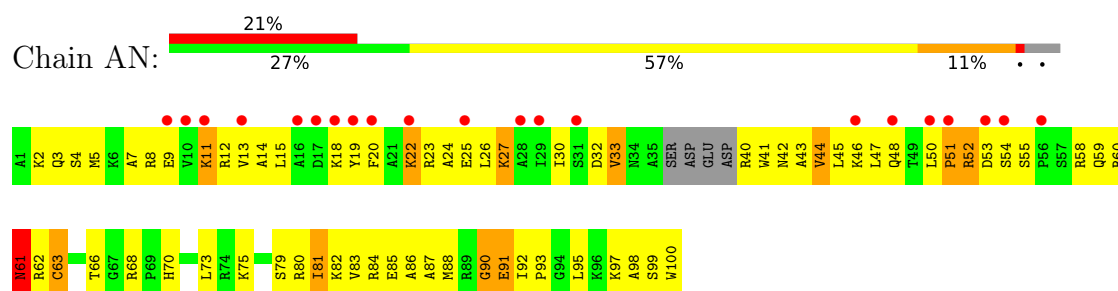
- Molecule 12: 30S ribosomal protein S12



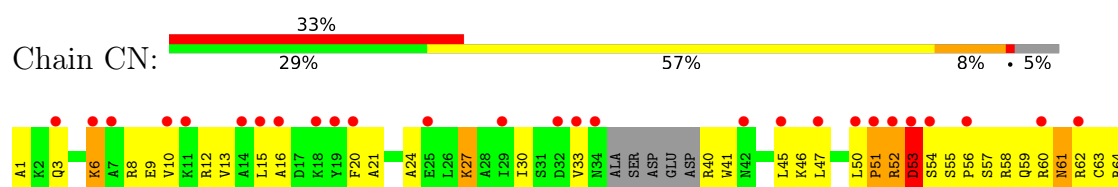
- Molecule 13: 30S ribosomal protein S13

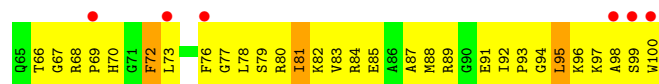


- Molecule 14: 30S ribosomal protein S14

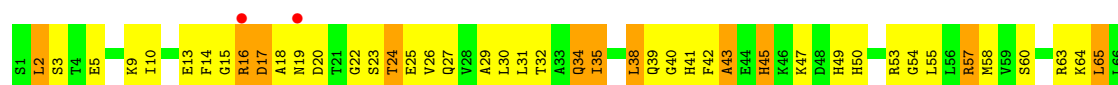


- Molecule 14: 30S ribosomal protein S14

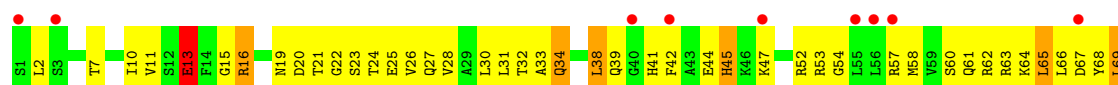




- Molecule 15: 30S ribosomal protein S15



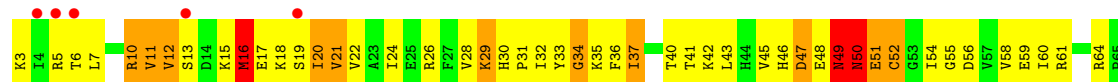
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

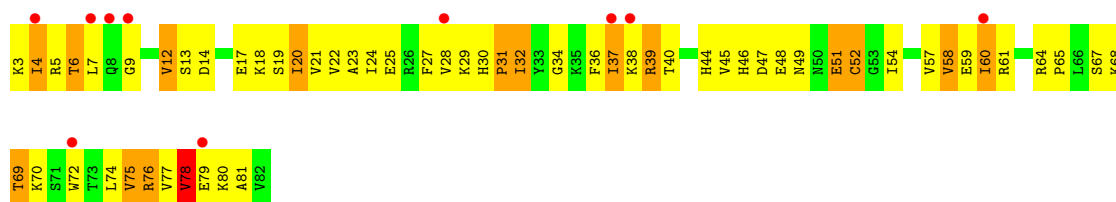


- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17

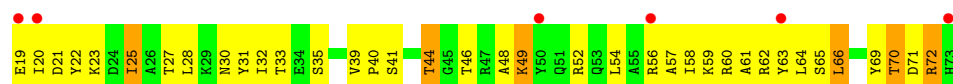




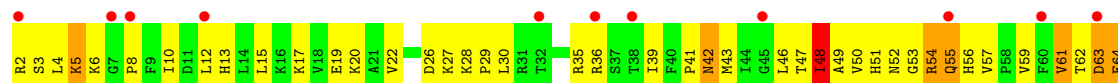
• Molecule 18: 30S ribosomal protein S18



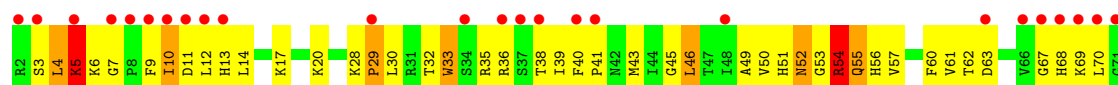
• Molecule 18: 30S ribosomal protein S18



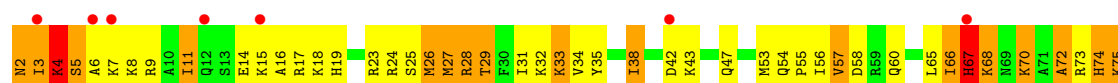
• Molecule 19: 30S ribosomal protein S19



• Molecule 19: 30S ribosomal protein S19

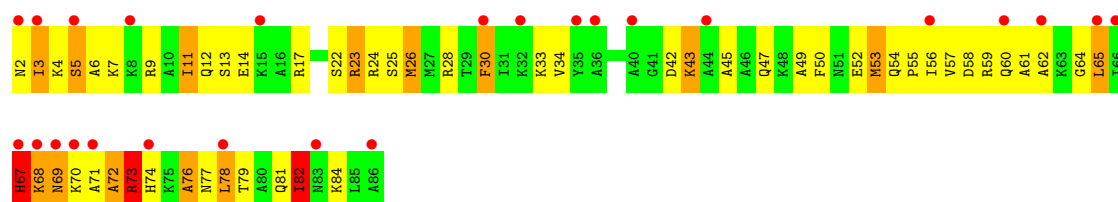


• Molecule 20: 30S ribosomal protein S20





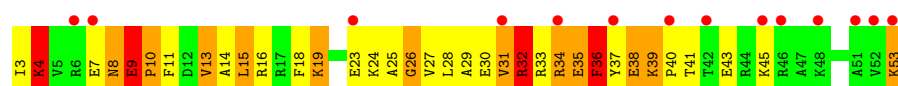
• Molecule 20: 30S ribosomal protein S20



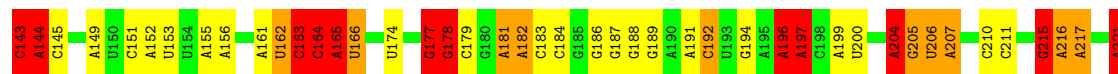
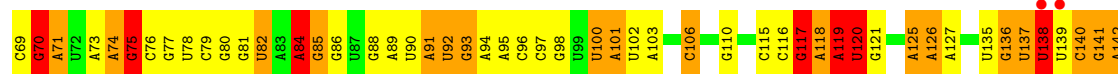
• Molecule 21: 30S ribosomal protein S21



• Molecule 21: 30S ribosomal protein S21

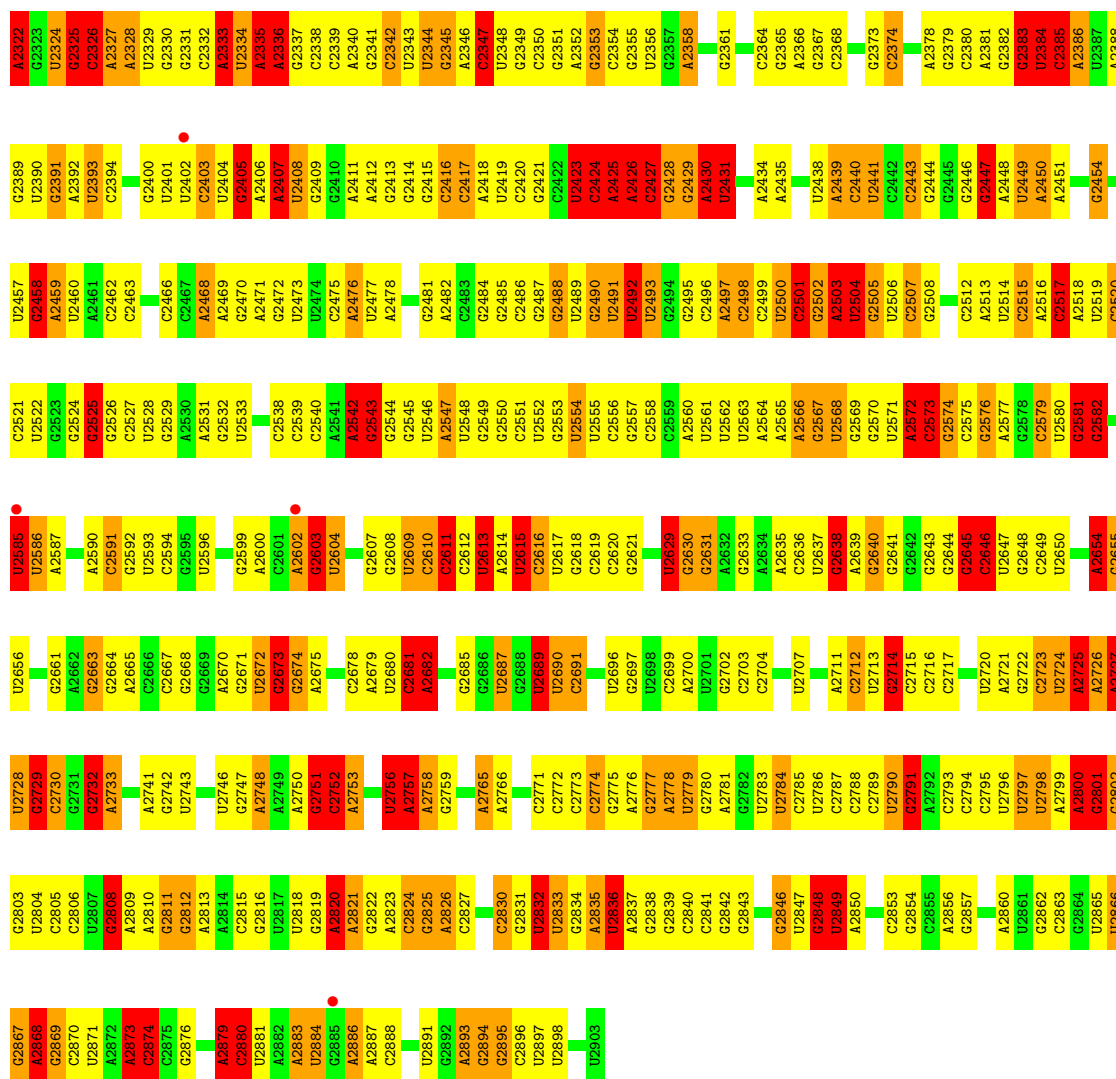


• Molecule 22: 23S rRNA

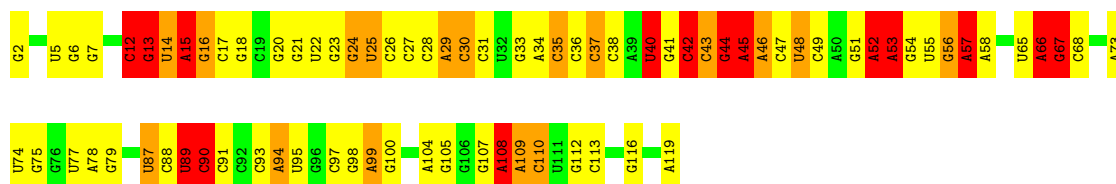


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C1296	G1167	U1035	G1166	G1099	U1036	G974	C908	U839	G774	A705	C634	C635	G494	G424	G359
C1297	G1168	G1036	C1187	A1103	G1036	A975	A909	U842	G775	A706	C635	G775	U587	G424	U360
C1298	G1169	A1039	G1168	C1104	A1039	G976	A910	U842	G776	A707	C636	G776	A497	A430	G361
C1299	G1170	A1040	C1170	G1105	A1040	G977	A911	G843	G777	A708	A638	G777	U588	U431	A362
G1238	G1171	G1041	C1171	G1106	G1041	G978	G912	G844	G778	U709	G638	G778	U499	G363	G363
G1239	C1172	G1042	C1172	G1107	G1042	A980	U913	A845	U779	U710	U639	U779	U571	C354	C354
U1240	A1175	C1043	G1175	A981	C1043	A981	C914	U846	G780	U714	C640	C640	A503	C435	U369
C1243	G1176	C1044	G1176	A982	C1044	A982	C915	U847	A781	A715	U641	U641	A504	C436	G370
A1244	G1177	C1045	G1177	A983	C1045	A983	C916	C848	A782	A716	U642	U642	A505	U441	A371
G1245	G1178	G1046	C1178	A984	G1046	A984	C917	C851	A783	A717	A643	A643	A506	G442	G372
A1246	G1179	G1047	C1179	C985	G1047	C985	A918	U851	G784	C717	A644	A644	A507	A443	U373
G1309	U1180	A1048	G1180	C986	A1048	C986	A920	C854	G786	C719	U646	U646	A508	C444	U374
G1310	U1181	C1049	G1181	C987	C1049	C987	C921	G855	C787	A722	G647	G647	A509	C445	A375
G1311	U1182	A1050	G1182	A988	C1050	A988	C922	G856	A788	A718	G648	G648	C581	G446	G375
U1312	G1183	G1116	C1183	G989	G1116	G989	G923	G857	A789	G726	U652	U652	C582	G376	G376
U1313	U1184	G1055	G1184	A990	G1055	A990	G924	G858	U790	G725	G651	G651	A512	U448	G377
C1314	G1185	G1056	C1185	C991	G1056	C991	G924	G859	C791	G726	U652	U652	A514	A449	C378
C1315	G1186	A1057	G1186	C992	A1057	C992	A928	U860	A792	A730	U653	U653	U519	G450	G379
U1316	U1187	U1058	U1187	G993	U1058	G993	U929	A861	A793	G727	U653	U653	A522	U451	G380
G1317	U1188	G1059	G1188	C994	G1059	C994	U930	G862	A794	G728	A654	A654	A522	G452	A382
U1318	G1189	U1060	C1189	C995	U1060	C995	U931	G863	C795	G729	A655	A655	A522	A453	G383
G1319	U1190	U1061	G1190	A996	U1061	A996	U932	C865	G799	A730	G656	G656	C523	A454	A384
C1320	G1191	G1062	C1191	G997	G1062	G997	U933	A866	G799	G733	U658	U658	A526	C455	A385
A1321	G1192	U1063	G1192	C998	U1063	C998	U934	C867	A800	G734	U659	U659	C527	C456	G386
A1322	G1193	G1064	G1193	U999	G1064	U999	C935	U868	G801	A735	G660	G660	C527	A457	U387
C1323	U1194	U1065	C1194	A1000	U1065	A1000	A936	G869	A802	G736	U661	U661	A529	G458	G388
G1324	G1195	U1066	G1195	A1001	U1066	A1001	C937	U870	U803	C737	U662	U662	A529	U459	G389
A1325	U1196	A1067	U1196	C1002	A1067	C1002	U941	U871	A804	G738	G664	G664	C530	C461	U390
U1326	G1197	G1068	G1197	U1003	G1068	U1003	A941	U872	G805	G739	U665	U665	C531	G462	A391
A1327	C1200	A1069	C1200	U1004	A1069	U1004	C942	U873	G806	A740	U666	U666	A532	C463	U395
A1328	U1203	U1070	U1203	C1005	U1070	C1005	A945	G875	C807	G741	A666	A666	A534	G464	G396
U1329	U1204	G1136	U1204	C1006	G1136	C1006	C946	C876	G808	U741	U667	U667	G534	G465	U397
G1330	G1205	U1071	G1205	C1007	U1071	C1007	A947	A877	G809	G745	A668	A668	G535	A466	U399
A1331	U1206	A1073	U1206	A1008	A1073	A1008	A948	A878	U810	U746	G669	G669	A538	G469	G400
G1332	G1207	G1074	G1332	A1009	G1074	A1009	C949	G879	U811	U747	C671	C671	C542	A472	U403
G1333	C1207	C1075	C1207	A1010	C1075	A1010	G950	G880	C812	U748	C672	C672	C543	G473	A404
G1334	U1210	U1076	U1210	G1011	U1076	G1011	C951	G881	U813	G749	C673	C673	C544	G474	U405
C1335	G1211	A1077	G1211	U1012	A1077	U1012	G954	U884	C816	A751	A675	A675	C545	C475	G406
A1336	G1212	C1078	A1336	C1013	C1078	C1013	U955	A	C817	A752	G681	G681	U545	G476	U407
G1337	U1213	U1079	U1213	U1014	U1079	U1014	U956	U	G818	A753	G682	G682	U546	G477	G408
G1338	A1214	U1080	A1214	G1015	U1080	G1015	G957	C	A819	U754	U683	U683	A547	A478	G409
U1340	G1215	U1082	U1340	G1016	U1082	G1016	C958	U	A820	U755	G684	G684	G548	A479	G410
G1341	U1216	U1083	G1341	G1017	U1083	G1017	U959	C	A821	U756	A685	A685	G549	G481	G411
A1342	U1217	A1084	A1342	U1019	A1084	U1019	A959	G	A822	G757	U686	U686	C550	A482	A412
G1343	C1152	A1085	C1152	A1020	A1085	A1020	C961	A892	C823	G758	C687	C687	G553	A483	C413
G1344	C1153	U1086	C1153	A1021	U1086	A1021	C962	C893	U824	U761	U688	U688	U554	A484	A415
U1282	G1154	G1087	U1282	G1022	G1087	G1022	U963	C894	A825	U762	A693	A693	U555	C485	U416
G1283	A1155	A1088	A1155	U1023	A1088	U1023	C964	U895	U826	G763	U694	U694	A556	C486	C417
A1286	G1156	U1223	A1286	G1024	U1223	G1024	C965	U896	U827	G764	G697	G697	C557	G489	U419
U1287	U1224	A1089	U1287	G1025	A1089	G1025	C966	A897	U828	G765	U698	U698	U558	C490	C420
G1288	G1157	U1090	G1288	G1026	U1090	G1026	C967	C898	U829	U766	C699	C699	U559	C491	A422
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G1290	U1159	C1092	G1290	A1028	U1159	A1028	C968	A900	G831	U768	U699	U699	C563		
C1291	G1160	G1093	C1291	U1028	G1093	U1028	C969	C901	U832	U769	A632	A632	C564		
U1291	C1161	U1094	U1291	G1031	U1094	G1031	C970	U906	G834	G770	U703	U703			
G1292	G1162	A1095	G1292	A1032	A1095	A1032	G971								
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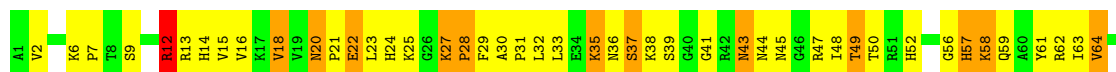
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C2260	U2184	G2055	G1986	U1917	G1840	G1776	G1707	G1568	G1432	A1359
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C2262	C2057	A2058	C1990	A1919	G1842	U1778	C1708	G1570	A1434	G1361
U2263	U2187	A2059	U1991	C1920	C1843	U1779	U1779	G1571	G1435	A1365
C2264	U2188	A2060	G1992	G1921	C1844	A1780	U1712	A1502	G1436	A1366
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A2267	A2063	C2064	C1997	C1924	G1849	A1783	U1715	A1505	A1439	U1373
C2268	C2065	G2066	A1998	C1925	G1850	A1784	G1716	U1506	U1440	G1374
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C2271	U2068	G2069	G2001	U1928	U1853	A1787	U1721	G1509	U1443	G1377
U2272	C2069	A2070	A2005	G1929	A1854	C1788	A1722	C1582	G1444	A1378
A2273	A2071	C2072	C2006	U1930	U1855	A1789	G1723	U1510	G1445	C1446
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C2297	C2093	A2032	A2038	G1961	A1886	U1818	A1754	U1549	U1476	U1412
U2298	U2105	U2034	U2039	C1962	A1889	U1820	A1755	C1550	A1413	A1414
C2299	U2106	G2035	C2036	U1963	A1890	A1821	G1756	A1551	U1415	U1415
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G2301	A2108	U2038	G2038	C1965	A1900	G1823	U1758	G1553	G1483	U1417
C2302	U2109	U2039	A1901	A1966	A1901	U1824	A1759	U1554	U1484	U1418
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U2306	U	C2044	A1970	U1971	G1907	A1828	G1763	C1558	G1488	G1422
C2307	A	C2045	A1971	C1972	C1908	A1829	U1764	G1559	C1489	U1423
G2308	C	G2046	U1972	G1980	C1909	C1832	G1765	G1560	A1490	G1423
A2309	A	C2047	U1980	A1981	U1910	U1833	G1766	G1561	G1491	G1426
C2310	U	G2048	A1982	U1982	U1911	U1834	U1769	U1562	C1492	G1427
U2311	G	C2049	U1983	U1984	A1912	G1836	G1770	U1563	C1493	A1428
G2312	A	C2050	A1913	G1984	A1913	C1837	G1771	G1564	A1494	A1429
C2313	G	A2052	C1914							
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G2315										
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C2317										
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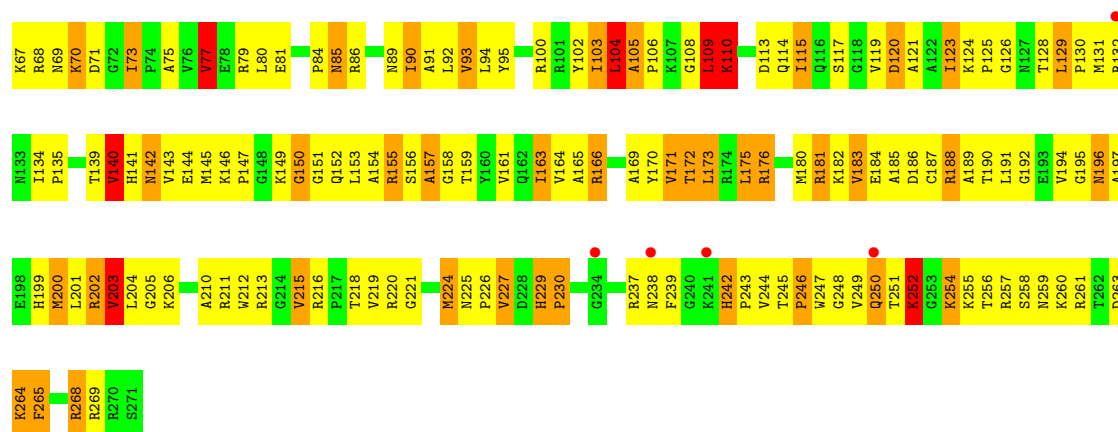


Chain BB:

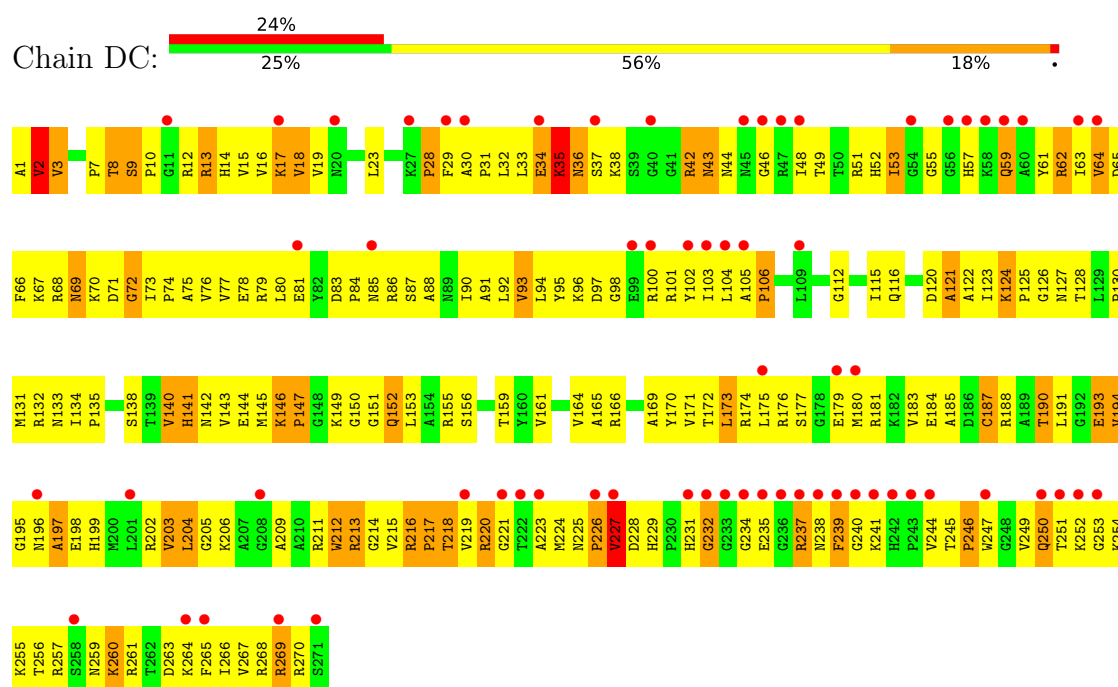


Chain BC:

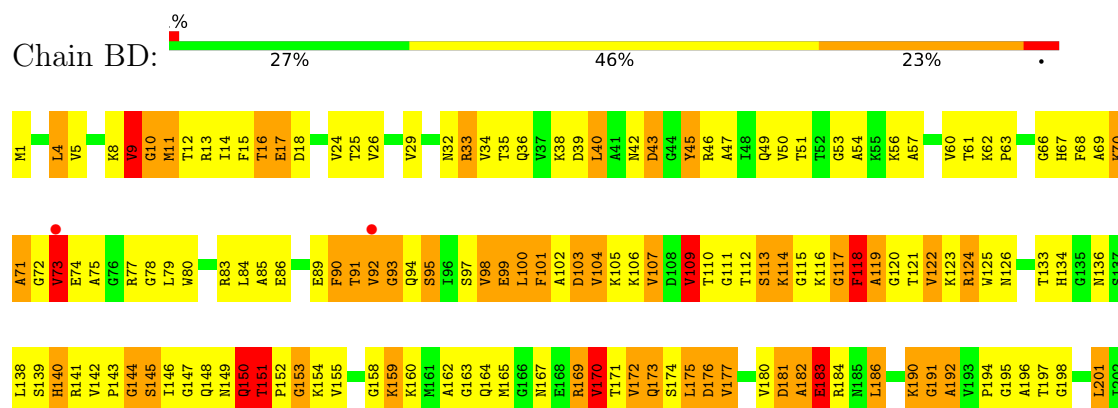




• Molecule 24: 50S ribosomal protein L2

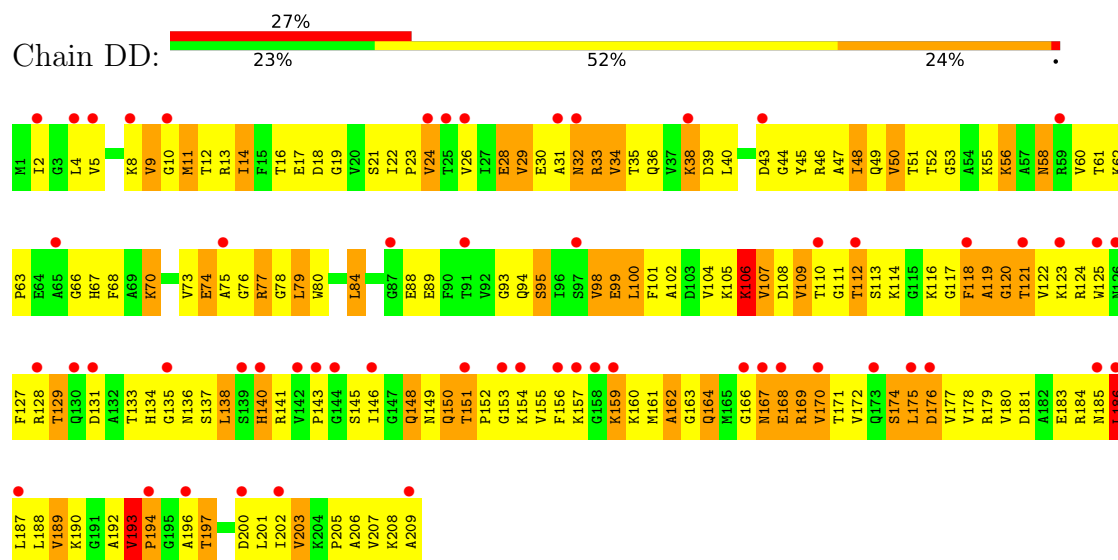


• Molecule 25: 50S ribosomal protein L3

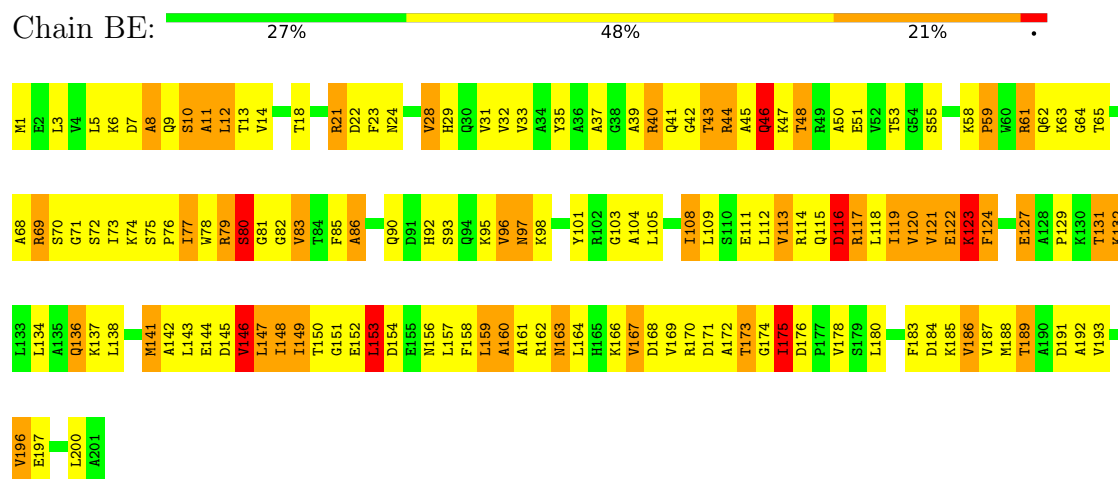




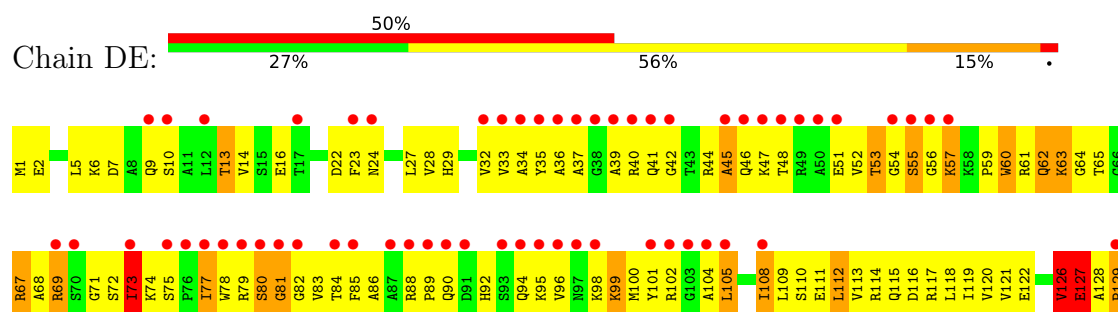
• Molecule 25: 50S ribosomal protein L3

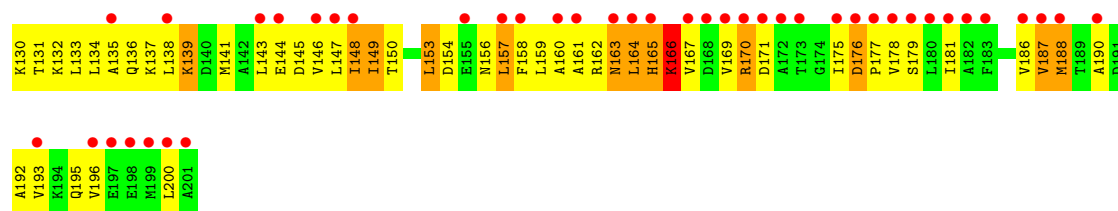


• Molecule 26: 50S ribosomal protein L4

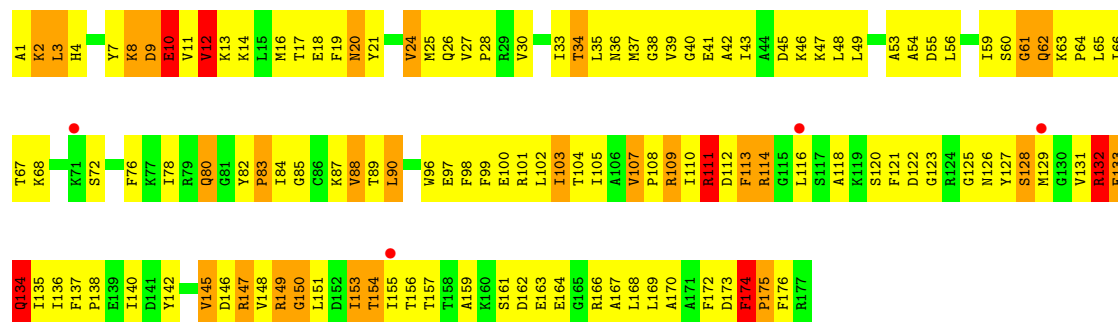


• Molecule 26: 50S ribosomal protein L4

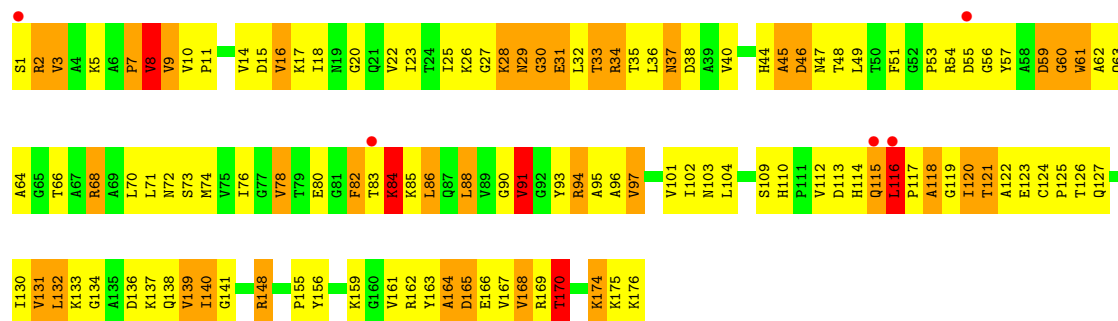




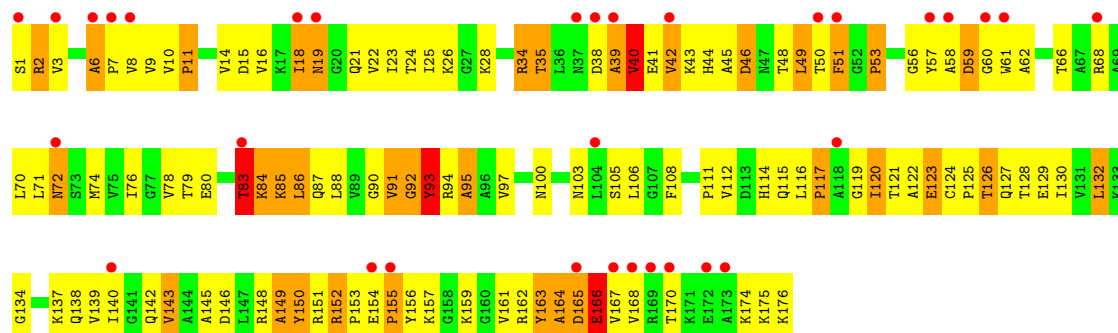
• Molecule 27: 50S ribosomal protein L5



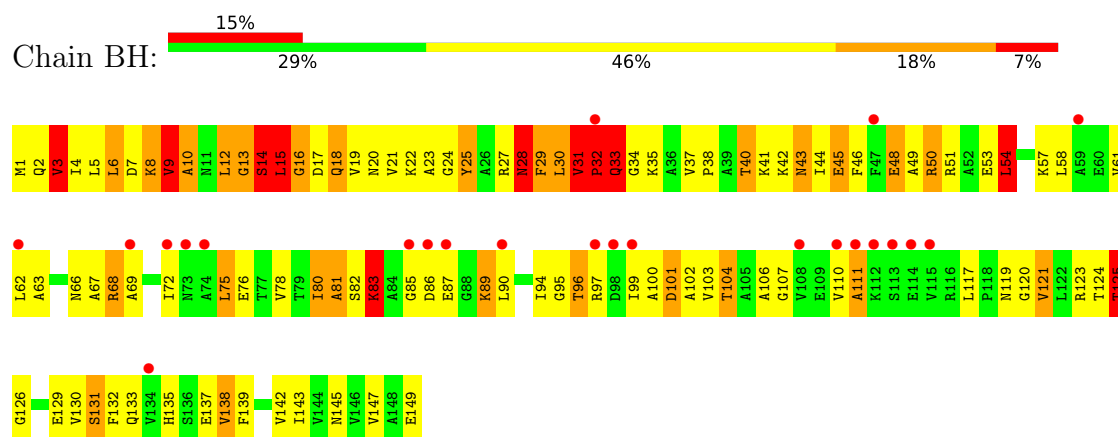
• Molecule 28: 50S ribosomal protein L6



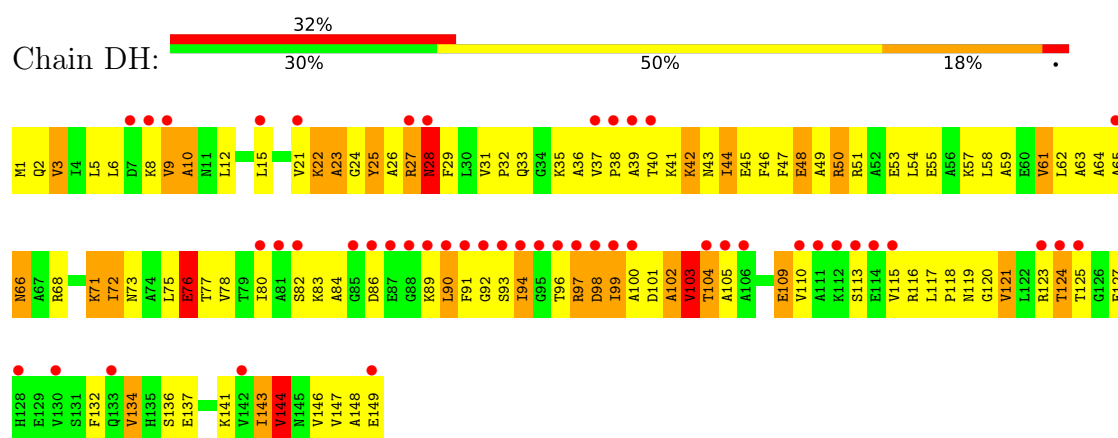
• Molecule 28: 50S ribosomal protein L6



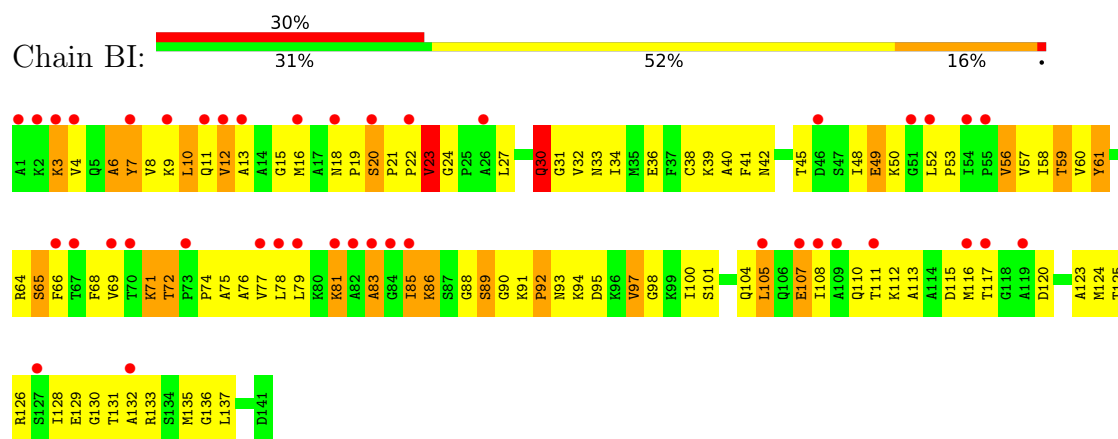
• Molecule 29: 50S ribosomal protein L9



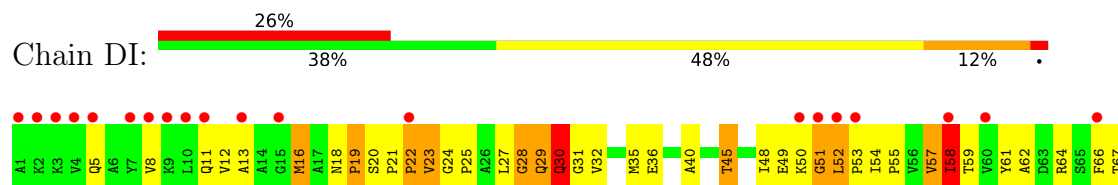
• Molecule 29: 50S ribosomal protein L9

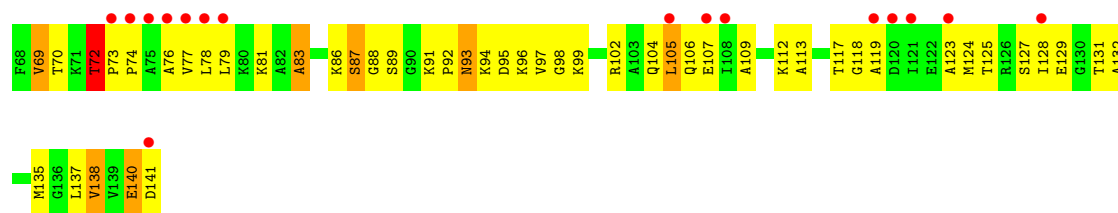


• Molecule 30: 50S ribosomal protein L11

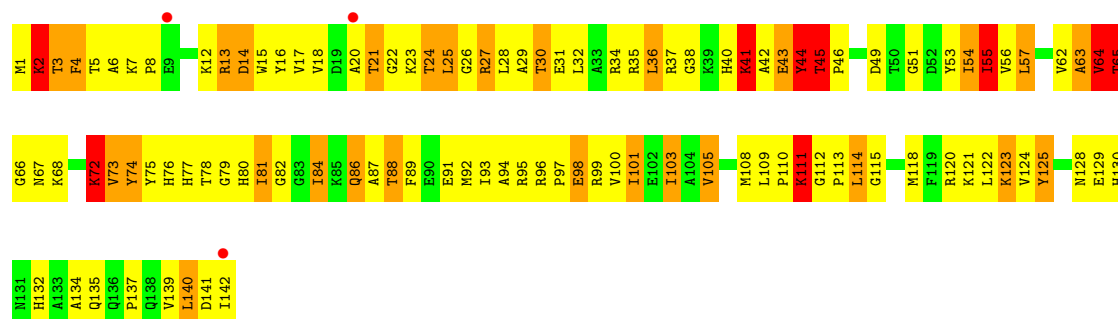


• Molecule 30: 50S ribosomal protein L11

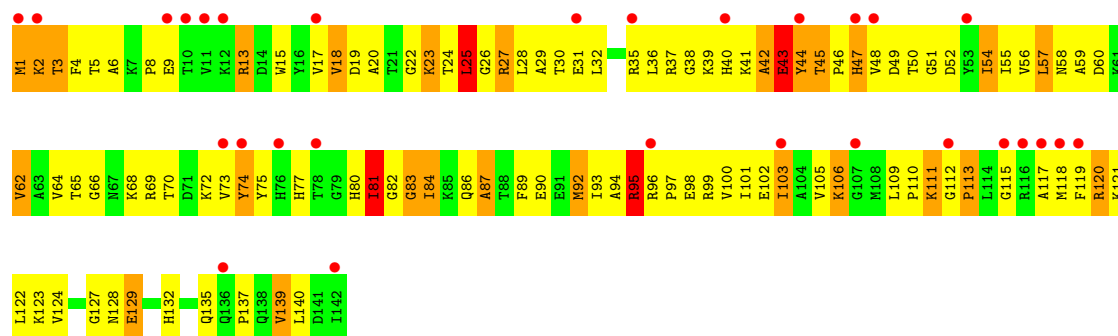




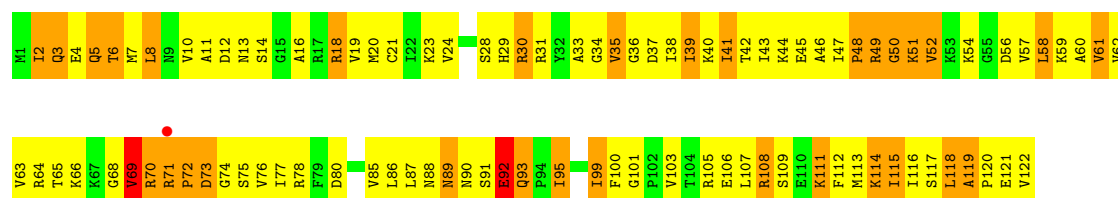
• Molecule 31: 50S ribosomal protein L13



• Molecule 31: 50S ribosomal protein L13

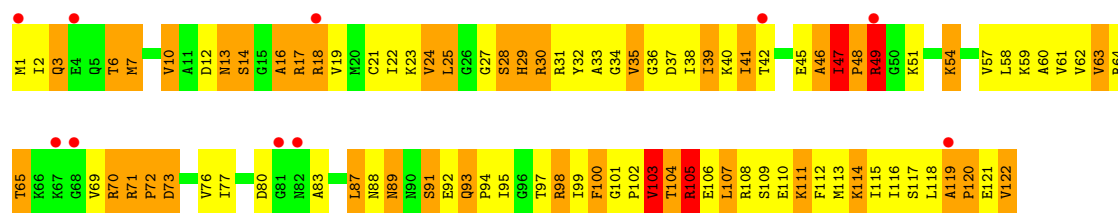


• Molecule 32: 50S ribosomal protein L14

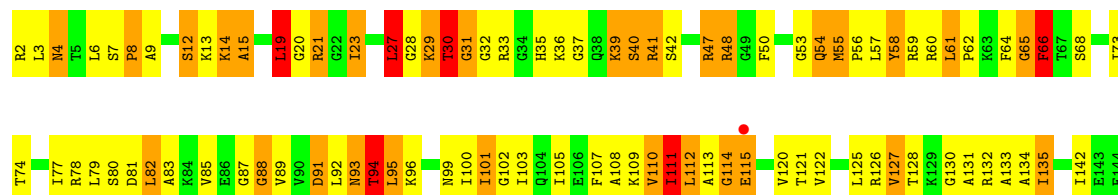


• Molecule 32: 50S ribosomal protein L14

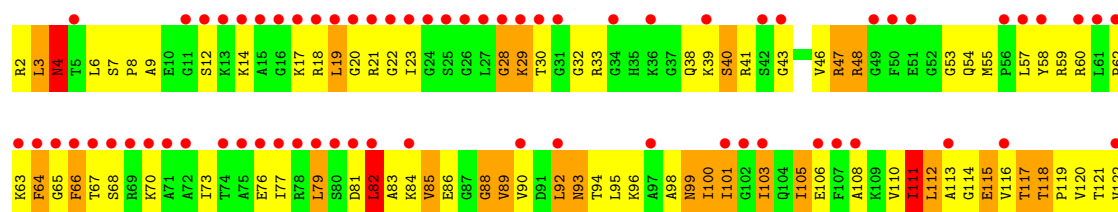




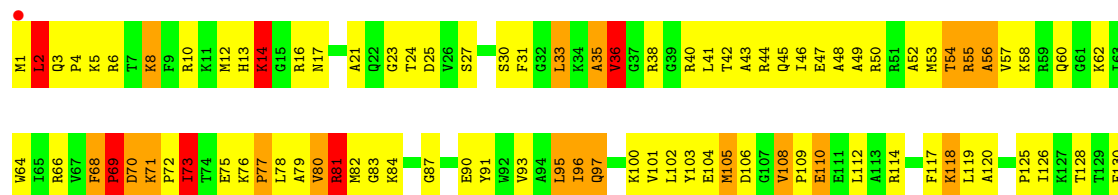
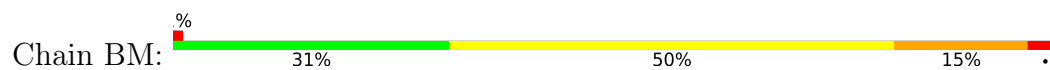
• Molecule 33: 50S ribosomal protein L15



• Molecule 33: 50S ribosomal protein L15

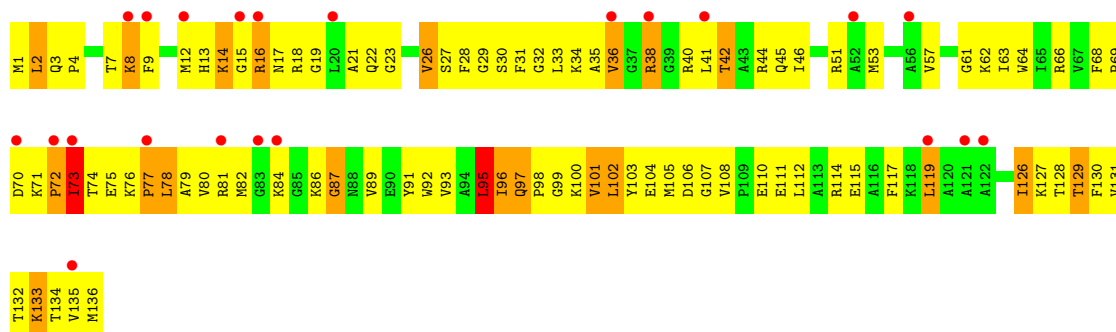


• Molecule 34: 50S ribosomal protein L16



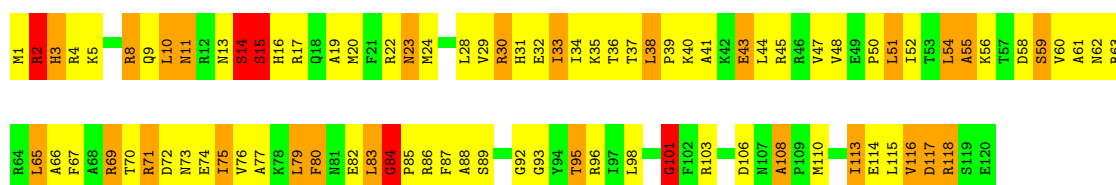
• Molecule 34: 50S ribosomal protein L16





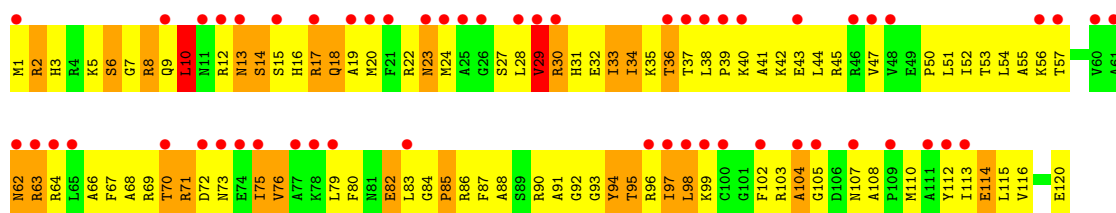
• Molecule 35: 50S ribosomal protein L17

Chain BN: 27% 48% 22% .



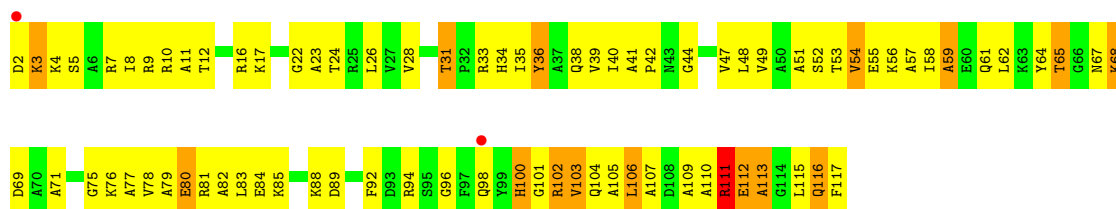
• Molecule 35: 50S ribosomal protein L17

Chain DN: 47% 22% 55% 22% .



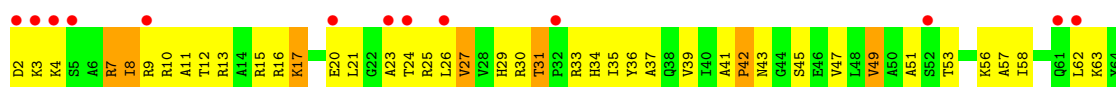
• Molecule 36: 50S ribosomal protein L18

Chain BO: 2% 30% 56% 13% .



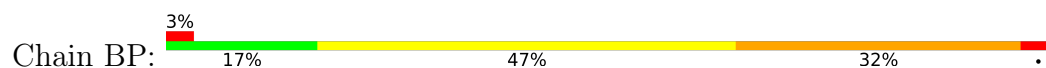
• Molecule 36: 50S ribosomal protein L18

Chain DO: 12% 40% 51% 9% .

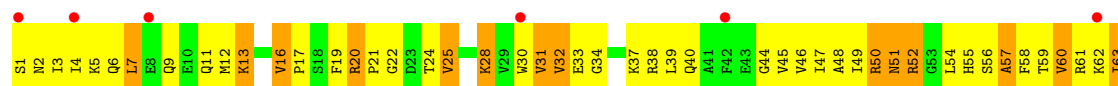




• Molecule 37: 50S ribosomal protein L19



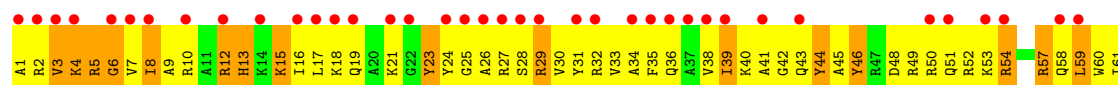
• Molecule 37: 50S ribosomal protein L19



• Molecule 38: 50S ribosomal protein L20

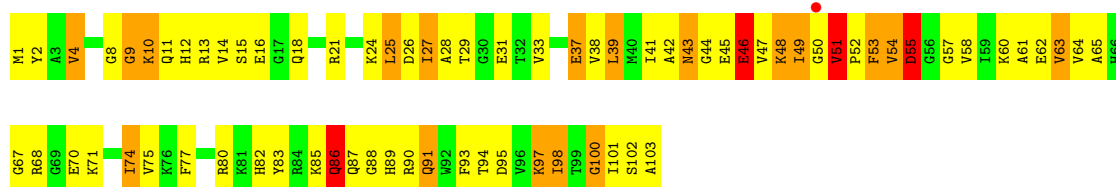


• Molecule 38: 50S ribosomal protein L20

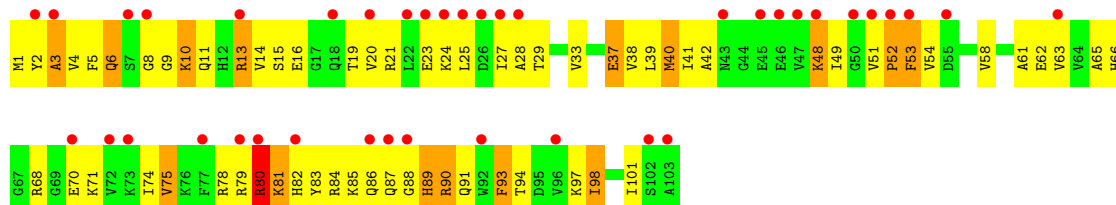


• Molecule 39: 50S ribosomal protein L21

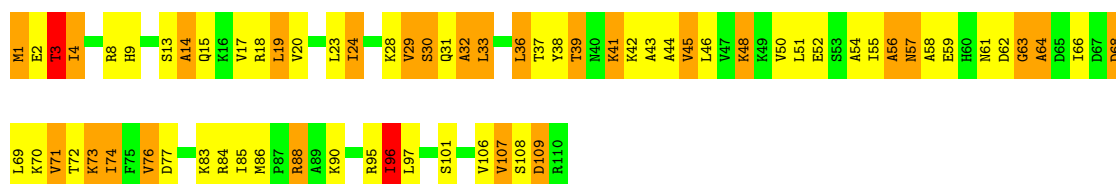




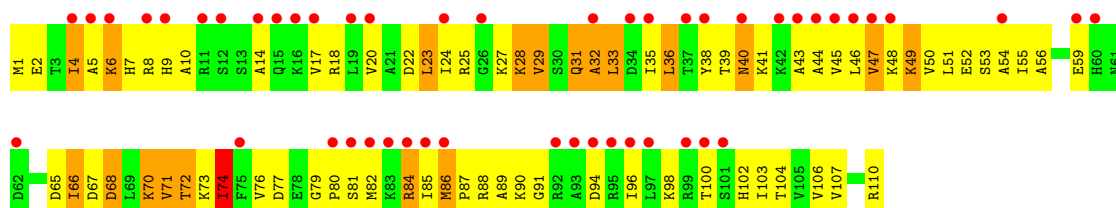
• Molecule 39: 50S ribosomal protein L21



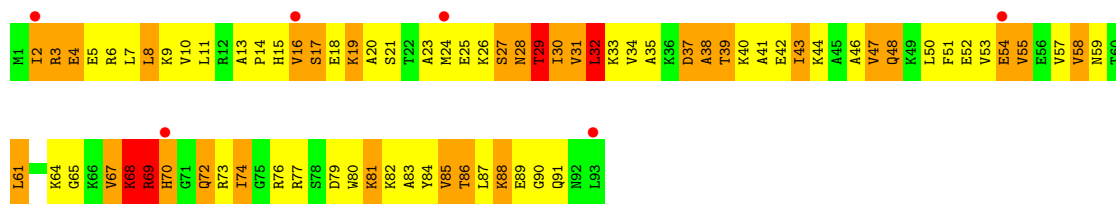
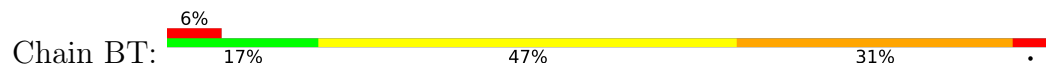
• Molecule 40: 50S ribosomal protein L22



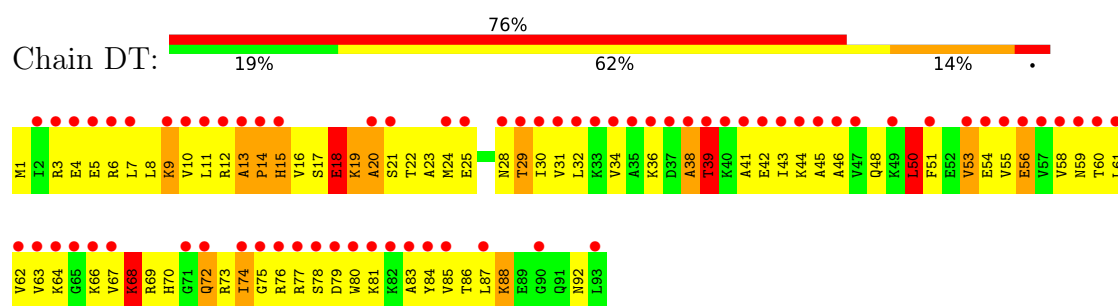
• Molecule 40: 50S ribosomal protein L22



• Molecule 41: 50S ribosomal protein L23



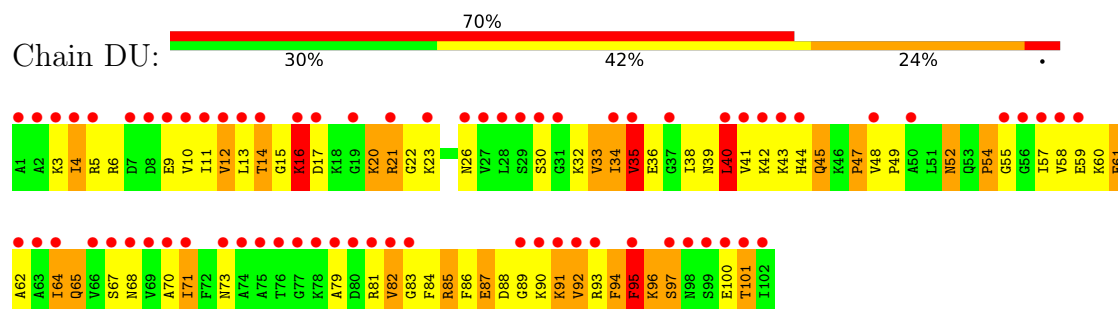
• Molecule 41: 50S ribosomal protein L23



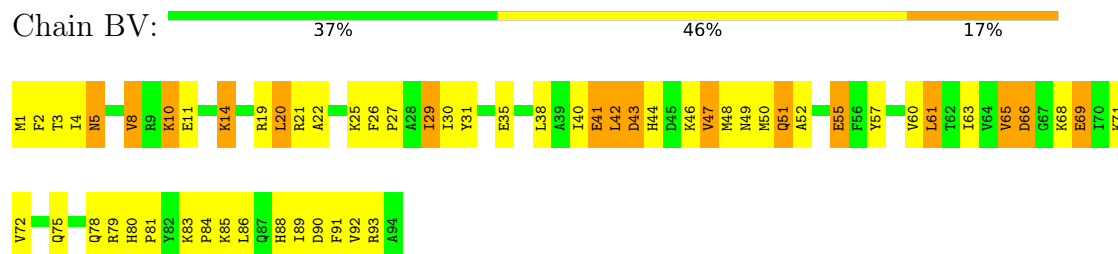
• Molecule 42: 50S ribosomal protein L24



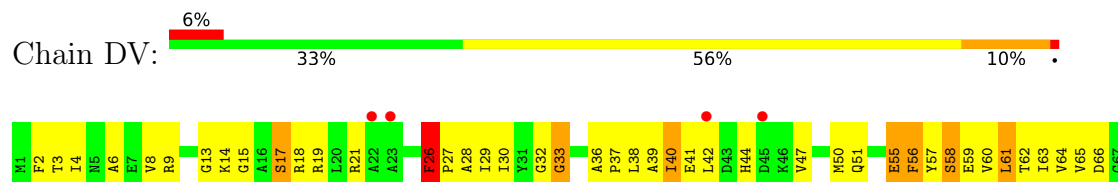
• Molecule 42: 50S ribosomal protein L24



• Molecule 43: 50S ribosomal protein L25

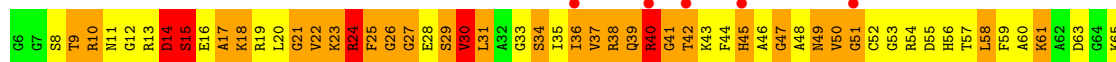


• Molecule 43: 50S ribosomal protein L25

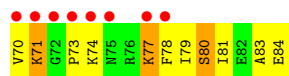
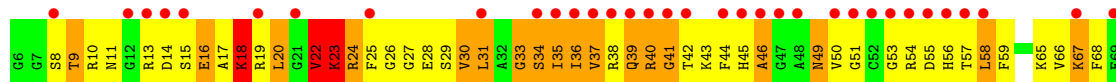




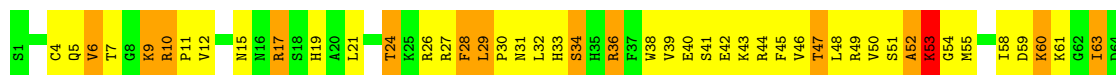
- Molecule 44: 50S ribosomal protein L27



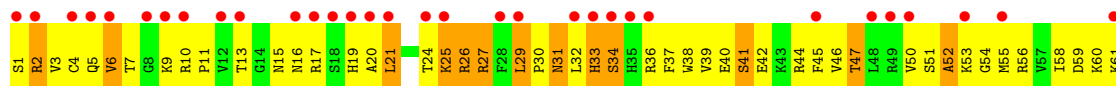
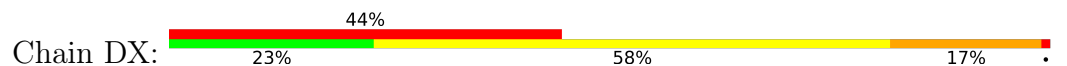
- Molecule 44: 50S ribosomal protein L27



- Molecule 45: 50S ribosomal protein L28

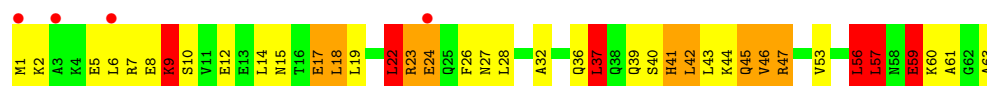


- Molecule 45: 50S ribosomal protein L28

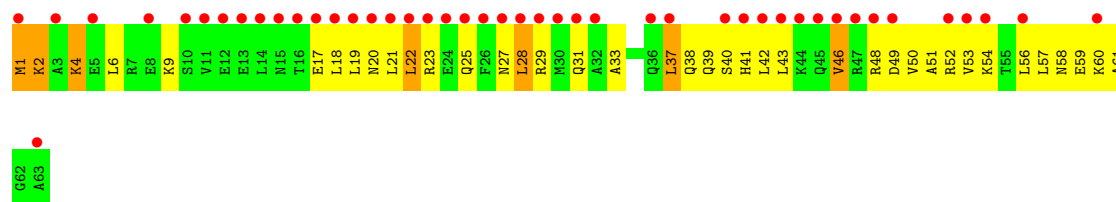
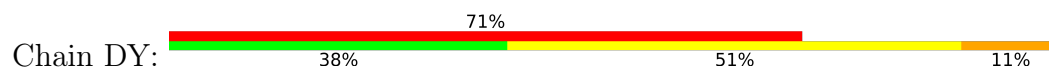


- Molecule 46: 50S ribosomal protein L29





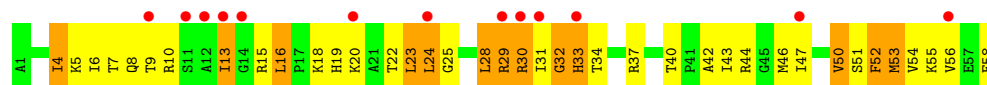
- Molecule 46: 50S ribosomal protein L29



- Molecule 47: 50S ribosomal protein L30



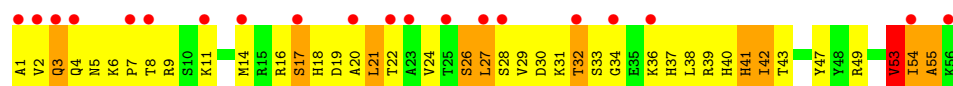
- Molecule 47: 50S ribosomal protein L30



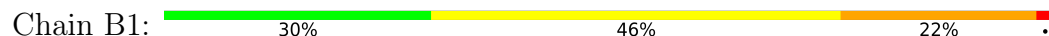
- Molecule 48: 50S ribosomal protein L32



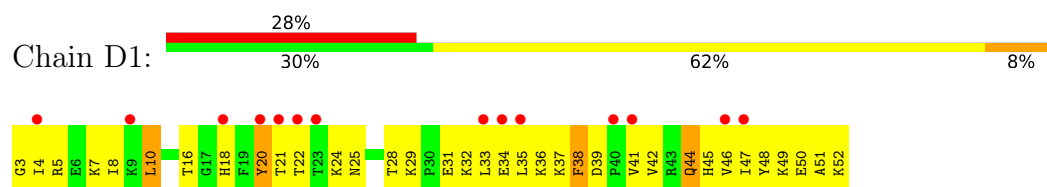
- Molecule 48: 50S ribosomal protein L32



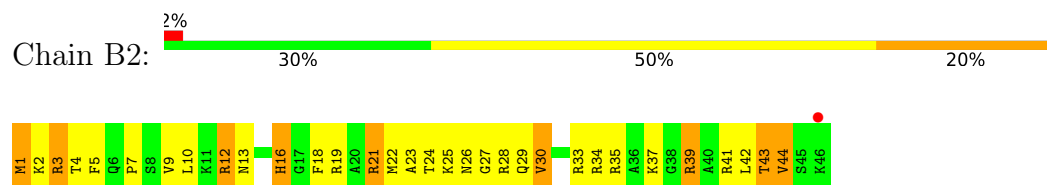
- Molecule 49: 50S ribosomal protein L33



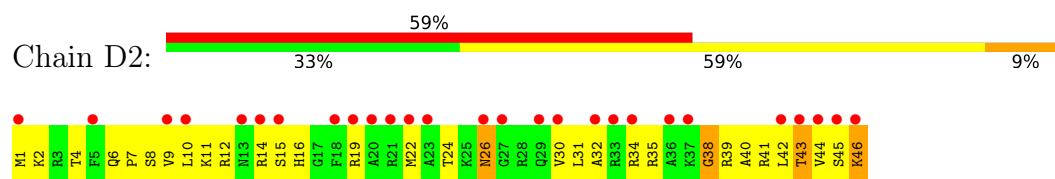
- Molecule 49: 50S ribosomal protein L33



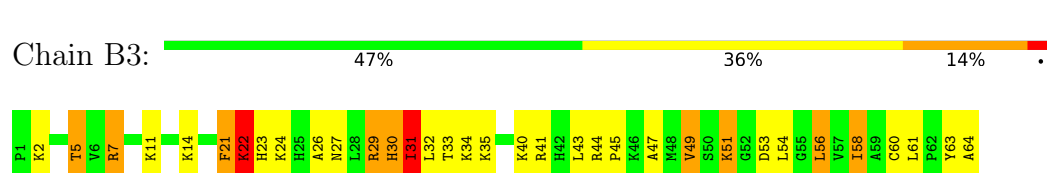
- Molecule 50: 50S ribosomal protein L34



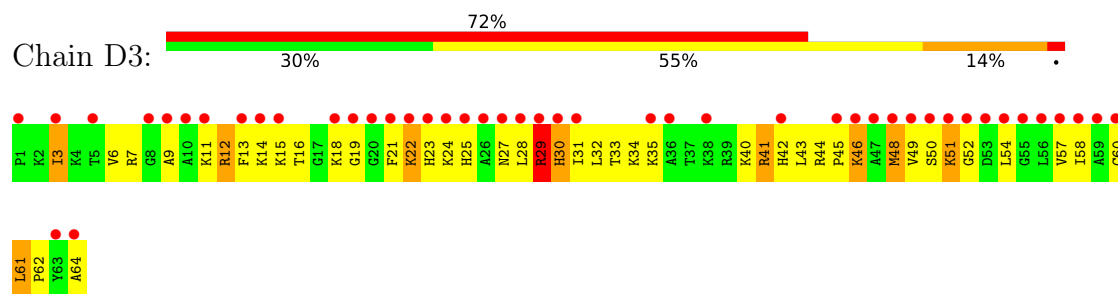
- Molecule 50: 50S ribosomal protein L34



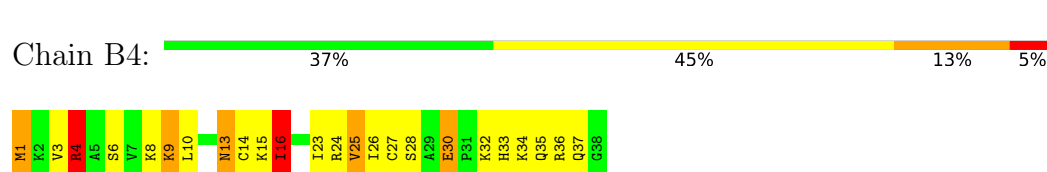
- Molecule 51: 50S ribosomal protein L35



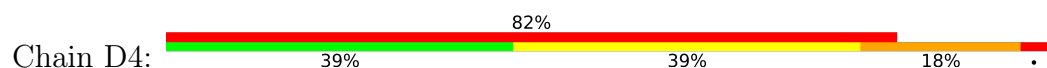
- Molecule 51: 50S ribosomal protein L35

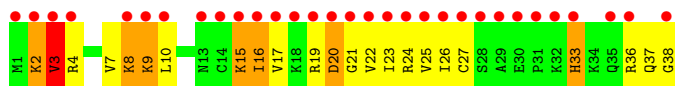


- Molecule 52: 50S ribosomal protein L36

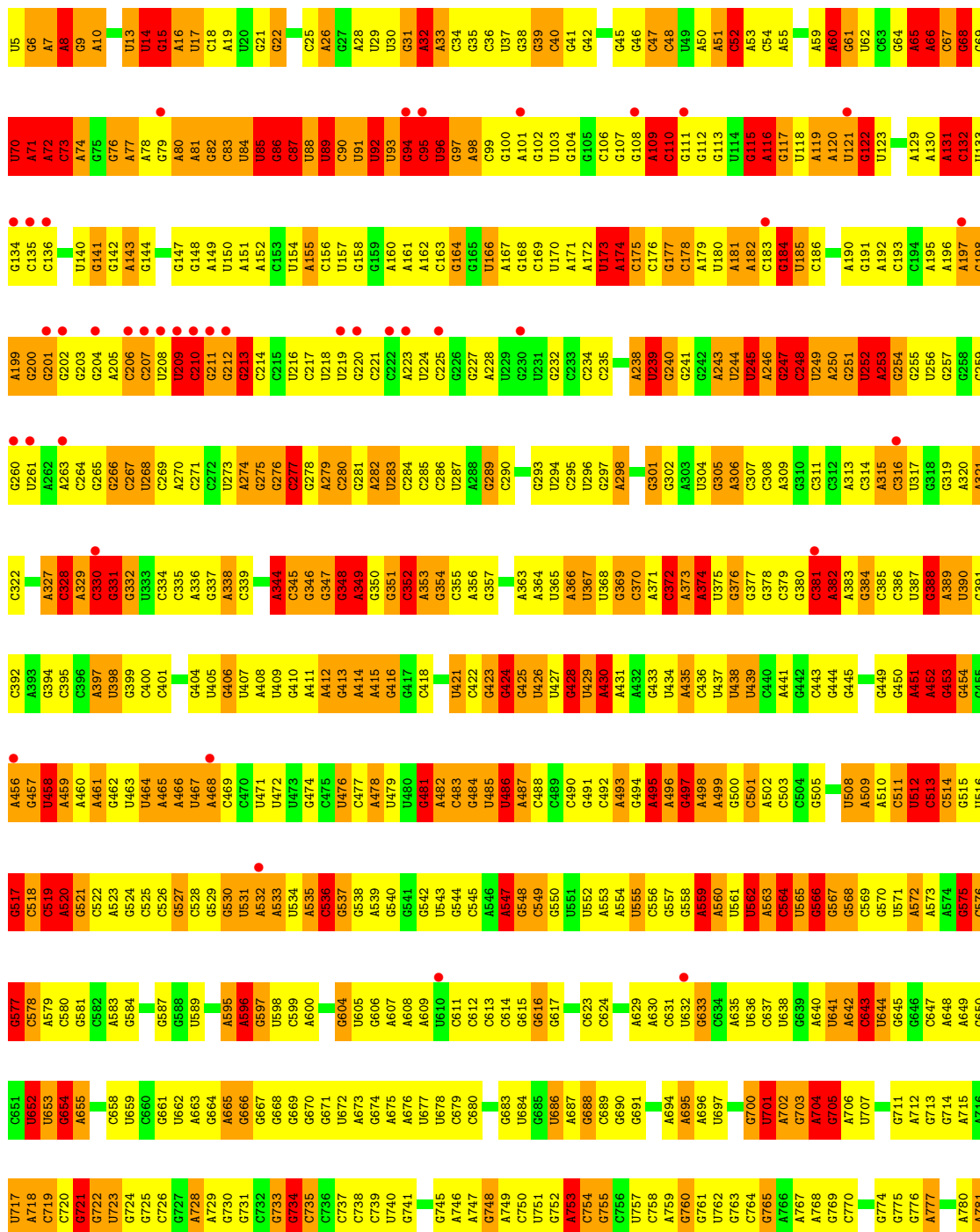
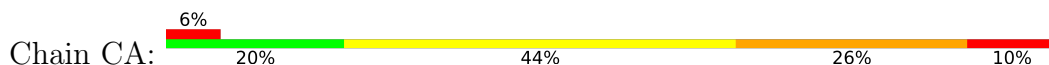


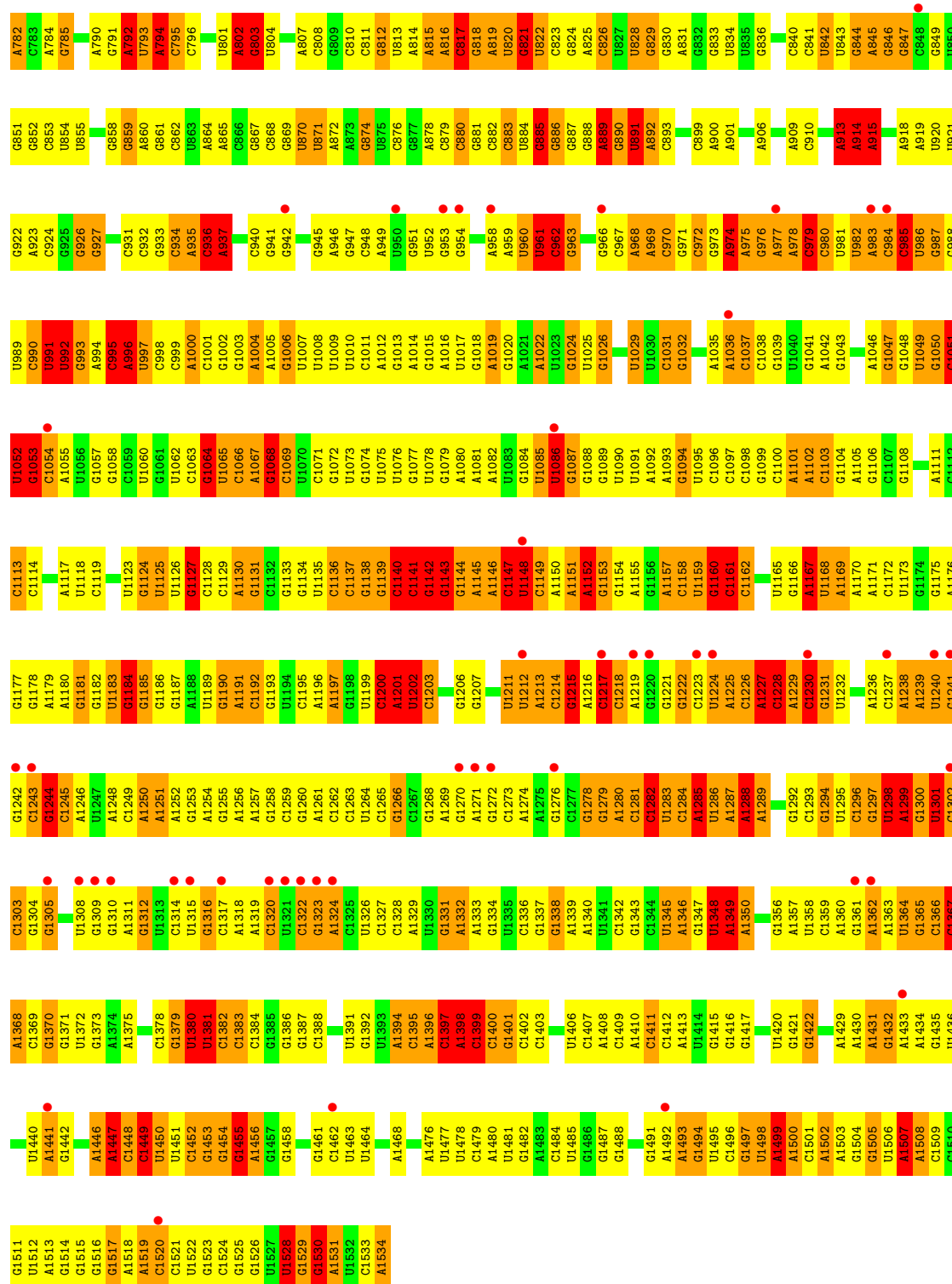
- Molecule 52: 50S ribosomal protein L36



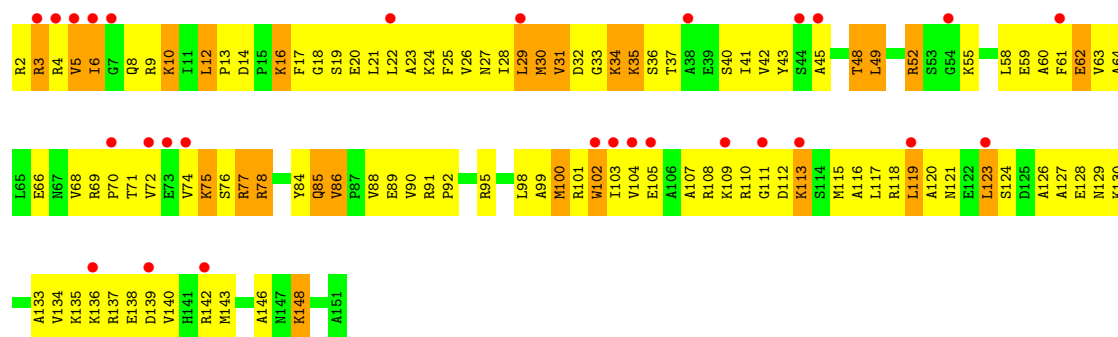


● Molecule 53: 16S rRNA

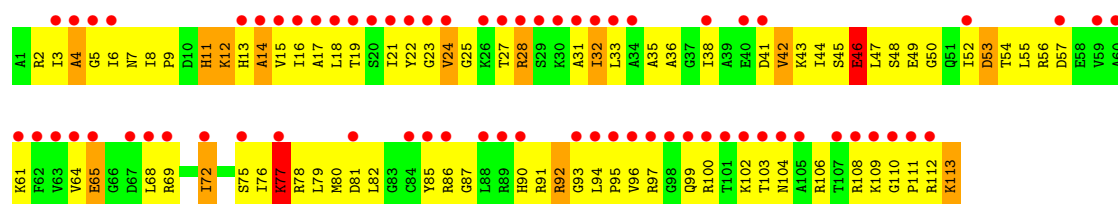




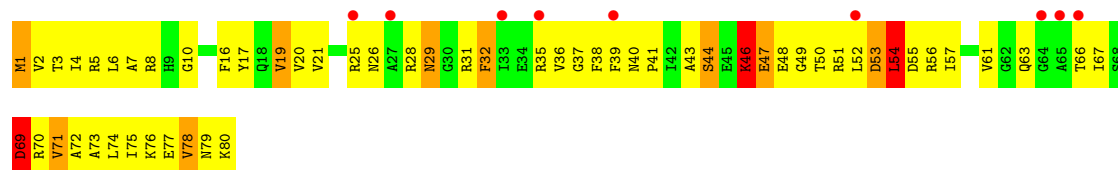
• Molecule 54: 30S ribosomal protein S7



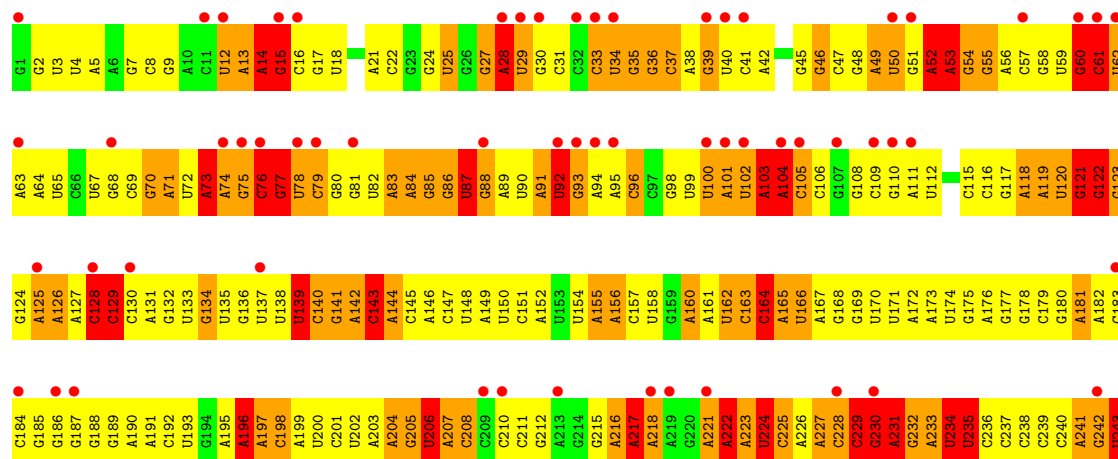
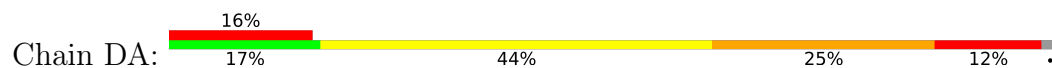
• Molecule 55: 30S ribosomal protein S13

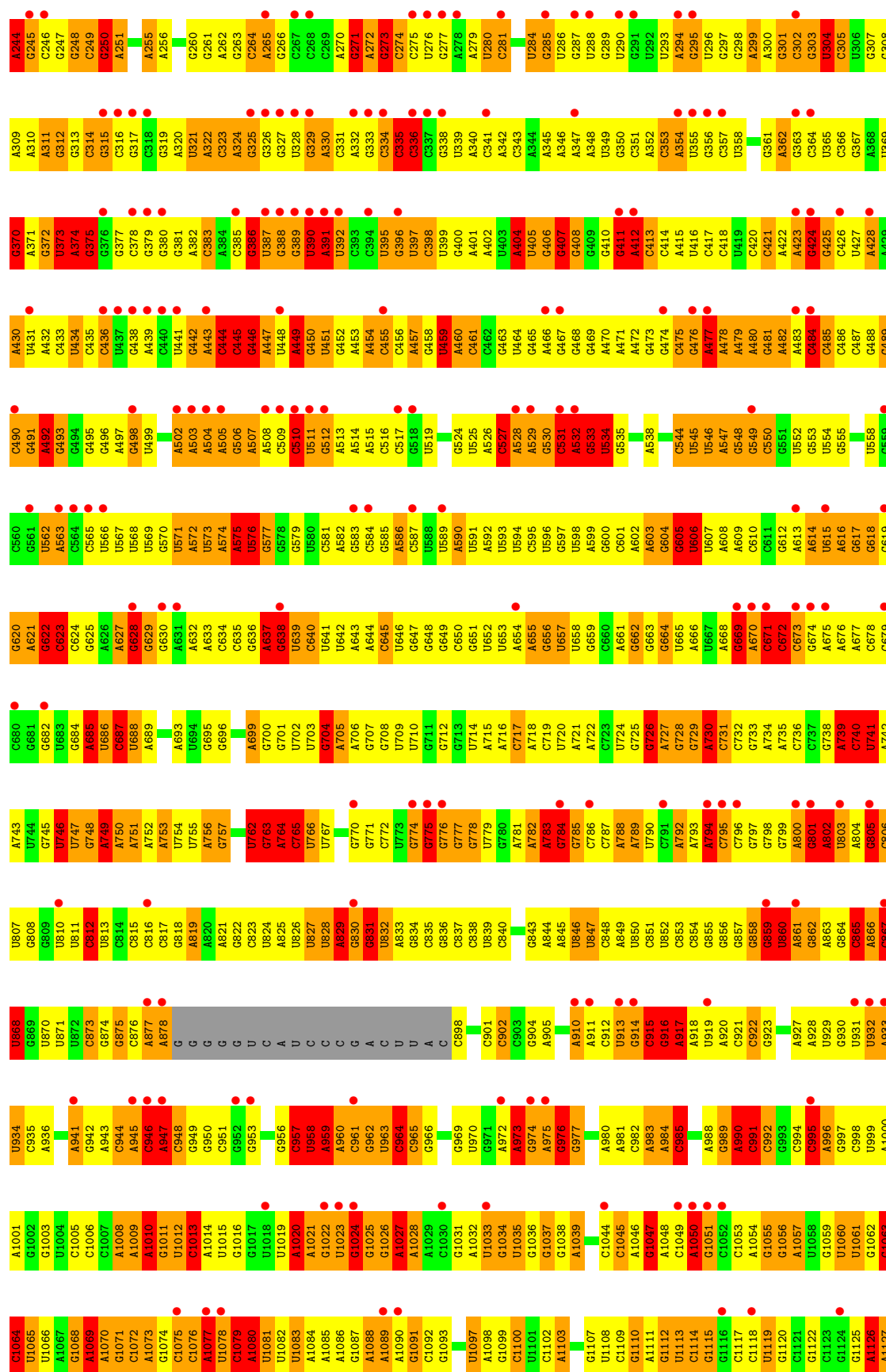


• Molecule 56: 30S ribosomal protein S16



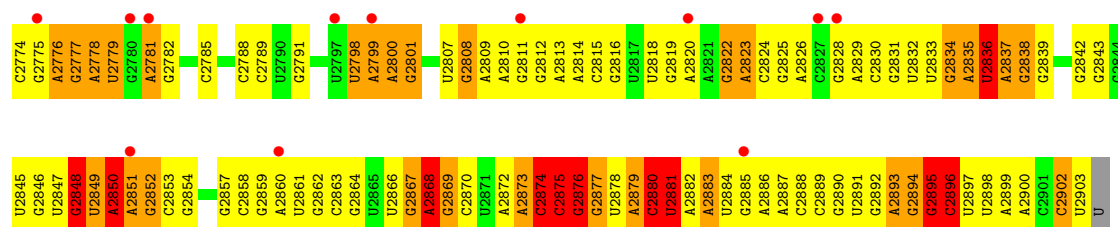
• Molecule 57: 23S rRNA



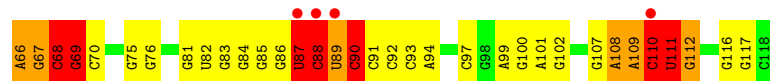
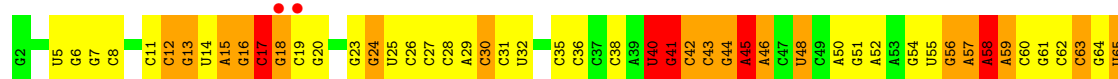




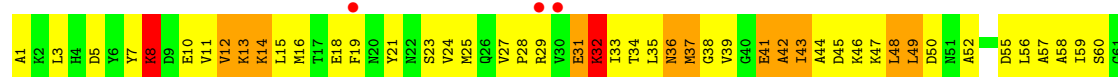
C2712	U2850	C2520	U2456	U2391	U2324	C2263	A2199	G2138	U2074	A2014	U1944
U2713	C2651	C2521	U2457	A2392	C2325	C2264	C2200	U2139	U2075	A2015	G1945
C2714	A2587	G2525	G2463	U2393	G2326	U2265	U2202	G2140	A2076	U2016	U1946
U2715	A2589	G2526	G2464	C2394	A2327	C2266	G2203	G2141	A2077	U2017	
C2716	A2590	C2527	C2465	U2395	U2328	A2267	U2204	C2142		G2018	U1951
U2717	U2591	C2527	C2466	G2396	U2329	A2268	G2204	A2143	A2080	A2019	A1952
C2718	U2593	U2598	C2467	G2397	G2330	G2269		C2144	U2081	A2020	A1953
U2719	C2594	G2599	G2468	G2331	C2331	A2270	C2207	C2145	A2082	C2021	G1964
C2720	U2595	A2530	U2401	C2332	C2332	U2271	C2208	C2146	G2083	U2022	U1956
A2721	U2596	U2533	U2402	A2333	U2333	U2272	C2209	A2147		C2023	C1957
C2722	C2597	U2533	C2403	U2334	U2334	U2273	U2210	A2148	A2088	G2024	
U2723	A2598	A2534	U2404	A2335	A2335	A2274	A2211	U2149	A2089	C2025	
C2724	C2599	U2537	G2405	A2336	A2336	G2275	A2212	C2150	A2090	U2026	G1962
A2725	U2600	U2537	A2406	G2337	G2337	G2276	U2213	U2151	C2091	G2027	U1963
U2726	C2601	C2538	A2407	C2338	U2338	A2277	C2214	U2152	U2092	U2028	G1964
C2727	A2602	C2539	U2408	C2339	G2340	A2278	C2215	C2153	G2093	U2029	C1965
U2728	U2603	U2540	G2409	A2340	A2340	G2279	C2216	U2154	A2094	C2030	A1966
C2729	U2604	A2542	U2475	G2410	G2341	G2280	G2217	U2155	A2095	A2031	G1967
U2730	U2605	G2543	A2476	A2411	C2342	A2281	U2218	G2156	C2096	G2032	A1968
C2731	C2606	G2544	U2477	U2412	U2343	G2282	C2219	G2157	A2097	A2033	A1969
U2732	G2607	U2545	A2478	G2413	U2344	C2283	U2220	A	U2098	U2034	A1970
A2733	U2608	U2546	U2479	G2414	G2345	A2284	G2221	G	U2099	G2035	U1971
C2734	U2609	A2547	C2480	G2415	A2346	C2285	C2222	C	G2100	C2036	G1972
U2735	G2610	U2548	G2481	C2416	C2347	G2286	G2223	C	A2101	A2037	G1973
C2736	C2611	G2549	C2417	C2417	U2348	A2287	G2224	G	G2102	U2038	C1974
U2737	C2612	C2550	A2418	U2418	G2349	A2288	A2225	A	C2103	U2039	G1975
C2738	U2613	C2551	A2419	C2420	C2350	G2289	U2226	A	C2104	G2040	
U2739	A2614	U2552	G2421	C2421	G2351	C2290	A2227	C	U2105	U2041	U1979
A2740	U2615	U2554	G2422	C2422	A2352	U2291	U2228	U	G2106	A2042	G1980
C2741	C2616	U2554	U2488	G2423	G2353	U2292	U2229	U	C2107	C2043	A1981
U2742	U2617	U2554	U2489	U2423	C2354	G2293	U2230	G	A2108	C2044	U1982
C2743	C2618	G2557	U2490	C2424	G2355	U2294	U2231	A	U2109	C2045	G1983
U2744	U2619	C2558	U2491	A2425	U2356	G2295	C2232	A	G2110	G2046	G1984
C2745	C2620	C2559	U2492	A2426	G2357	U2296	U2233	A	U	C2047	C1985
U2746	G2621	A2560	U2493	C2427	A2358	A2297	G2234	U	G	G2048	
C2747	U2561	U2562	G2428	G2428	C2359	A2298	U2235	A	U	G2049	C1986
U2748	G2623	U2562	G2429	G2429	G2360	U2299	U2236	C	A	C2050	
A2749	C2624	U2563	A2430	U2430	G2361	C2300	G2237	C	A	A2051	G1989
U2750	G2625		U2431	U2431			G2238	A	G	G2052	C1990
C2751	U2626	A2566	A2432	A2432	G2365	G2303	G2239	A	G	A2053	U1991
U2752	C2627	U2567	U2500	G2433	A2366	G2304	U2240	C	A	G2054	G1992
A2753	G2628	U2568	C2501	A2434	G2367	U2305	A2241		U	C2055	U1993
C2754	U2629	G2569	G2502	A2435	G2367	C2306	G2242		A	G2056	C1994
U2755	C2630	G2570	A2503	G2436	G2371	G2307	U2243		G	G2057	U1995
C2756	G2631	U2571	U2504	G2437	U2372	G2308	U2244		U	A2058	C1996
U2757	A2632	A2572	C2505	U2438	G2373	A2309	U2245		G	G2059	C1997
A2758	U2635	C2573	U2506	A2439	C2374	C2310			G	A2060	A1998
C2759	G2636	G2574	C2507	A2440	G2375	A2311	U2249		G	G2061	C2000
U2760	U2637	C2575	G2508	U2441	G2380	U2312	G2250		A	A2062	C2001
A2761	G2638	A2577	G2509	C2442	A2381	C2313	G2251		G	C2063	
	U2639	U2578	U2510	C2443	G2382	A2314	G2255		G	C2064	G2004
C2762	G2642	C2579	C2512	G2444	A2383	G2315	G2256		C	C2065	A2005
U2763	U2645	U2580	A2513	G2445	U2384	G2316	U2257		U	G2066	C2006
A2764	C2646	G2581	U2514	G2447	C2385	A2317	G2258		U	G2067	U2007
C2765	U2647	G2582	C2515	A2448	A2386	G2318	U2259		U	U2068	C2008
U2766	G2648	C2583	A2516	U2449	U2387	U2320	U2260			A2070	G2009
A2767	U2649	U2584	C2517	U2450	A2388	U2321	C2261			A2071	U2011
C2768	U2650	G2585	A2518	A2451	G2389	A2322	G2262			C2072	G2012
U2769		U2586	U2519		U2390	G2323				C2073	A2013



• Molecule 58: 5S rRNA



• Molecule 59: 50S ribosomal protein L5



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.46Å 434.08Å 621.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.15 – 3.19 82.15 – 3.19	Depositor EDS
% Data completeness (in resolution range)	75.8 (82.15-3.19) 75.8 (82.15-3.19)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 3.19Å)	Xtriage
Refinement program	PHENIX, PHENIX (phenix.refine)	Depositor
R, R_{free}	0.191 , 0.252 0.203 , 0.261	Depositor DCC
R_{free} test set	15290 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	62.8	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 84.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	284499	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CLM, ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.33	3/36834 (0.0%)	0.99	260/57462 (0.5%)
2	AB	0.63	2/1736 (0.1%)	0.90	12/2338 (0.5%)
2	CB	0.64	2/1736 (0.1%)	0.88	6/2338 (0.3%)
3	AC	0.34	0/1652	0.85	2/2225 (0.1%)
3	CC	0.33	0/1652	0.76	0/2225
4	AD	0.37	0/1665	0.83	3/2227 (0.1%)
4	CD	0.44	0/1665	0.85	3/2227 (0.1%)
5	AE	0.53	2/1119 (0.2%)	0.92	5/1504 (0.3%)
5	CE	0.44	1/1119 (0.1%)	0.85	1/1504 (0.1%)
6	AF	0.36	0/836	0.79	1/1128 (0.1%)
6	CF	0.36	0/836	0.79	1/1128 (0.1%)
7	AG	0.32	0/1196	0.83	0/1602
8	AH	0.38	0/989	0.96	4/1326 (0.3%)
8	CH	0.35	0/989	0.83	2/1326 (0.2%)
9	AI	0.29	0/1034	0.77	0/1375
9	CI	0.30	0/1034	0.74	1/1375 (0.1%)
10	AJ	0.34	0/797	0.82	2/1077 (0.2%)
10	CJ	0.32	0/797	0.82	3/1077 (0.3%)
11	AK	0.35	0/893	0.91	1/1205 (0.1%)
11	CK	0.33	0/893	0.90	2/1205 (0.2%)
12	AL	0.48	0/969	0.98	1/1300 (0.1%)
12	CL	0.56	1/969 (0.1%)	0.87	2/1300 (0.2%)
13	AM	0.32	0/893	0.79	0/1193
14	AN	0.34	0/785	0.81	3/1043 (0.3%)
14	CN	0.27	0/780	0.77	0/1036
15	AO	0.36	0/722	0.74	0/964
15	CO	0.33	0/722	0.73	0/964
16	AP	0.37	0/659	0.87	2/884 (0.2%)
17	AQ	0.41	0/658	0.88	2/881 (0.2%)
17	CQ	0.39	0/658	0.83	0/881
18	AR	0.37	0/463	0.85	0/621
18	CR	0.35	0/463	0.77	0/621

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	AS	0.30	0/653	0.80	0/877
19	CS	0.26	0/653	0.83	2/877 (0.2%)
20	AT	0.39	0/671	0.91	3/888 (0.3%)
20	CT	0.33	0/671	0.88	3/888 (0.3%)
21	AU	0.35	0/431	0.85	0/570
21	CU	0.37	0/431	0.87	0/570
22	BA	0.43	2/68626 (0.0%)	1.14	760/107056 (0.7%)
23	BB	0.40	0/2828	1.11	30/4410 (0.7%)
24	BC	0.52	0/2122	1.05	14/2852 (0.5%)
24	DC	0.38	0/2122	0.89	5/2852 (0.2%)
25	BD	0.63	0/1586	1.16	7/2134 (0.3%)
25	DD	0.37	0/1586	0.93	7/2134 (0.3%)
26	BE	0.53	0/1571	0.98	8/2113 (0.4%)
26	DE	0.33	0/1571	0.80	2/2113 (0.1%)
27	BF	0.41	0/1435	0.89	4/1926 (0.2%)
28	BG	0.44	0/1343	0.95	5/1816 (0.3%)
28	DG	0.31	0/1343	0.79	2/1816 (0.1%)
29	BH	0.43	1/1122 (0.1%)	0.83	4/1515 (0.3%)
29	DH	0.52	1/1122 (0.1%)	0.77	1/1515 (0.1%)
30	BI	0.35	0/1046	0.88	4/1410 (0.3%)
30	DI	0.32	0/1046	0.85	3/1410 (0.2%)
31	BJ	0.70	1/1152 (0.1%)	1.23	13/1551 (0.8%)
31	DJ	0.36	0/1152	0.91	2/1551 (0.1%)
32	BK	0.61	0/948	1.06	1/1268 (0.1%)
32	DK	0.37	0/948	0.87	2/1268 (0.2%)
33	BL	0.59	1/1054 (0.1%)	1.09	5/1403 (0.4%)
33	DL	0.33	0/1054	0.81	0/1403
34	BM	0.56	0/1093	1.06	8/1460 (0.5%)
34	DM	0.34	0/1093	0.85	2/1460 (0.1%)
35	BN	0.59	0/974	1.03	7/1301 (0.5%)
35	DN	0.37	0/974	0.89	2/1301 (0.2%)
36	BO	0.52	0/902	0.93	2/1209 (0.2%)
36	DO	0.30	0/902	0.74	0/1209
37	BP	0.54	0/929	1.04	7/1242 (0.6%)
37	DP	0.36	0/929	0.89	5/1242 (0.4%)
38	BQ	0.69	0/960	1.09	6/1278 (0.5%)
38	DQ	0.34	0/960	0.76	0/1278
39	BR	0.63	0/829	1.09	6/1107 (0.5%)
39	DR	0.31	0/829	0.71	0/1107
40	BS	0.70	0/864	1.02	0/1156
40	DS	0.38	0/864	0.82	0/1156
41	BT	0.56	0/745	1.05	6/994 (0.6%)
41	DT	0.31	0/745	0.80	1/994 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
42	BU	0.52	0/788	1.13	8/1051 (0.8%)
42	DU	0.33	0/788	0.86	2/1051 (0.2%)
43	BV	0.51	0/766	0.89	0/1025
43	DV	0.31	0/766	0.80	2/1025 (0.2%)
44	BW	0.69	0/603	1.09	3/797 (0.4%)
44	DW	0.30	0/603	0.74	0/797
45	BX	0.52	0/635	0.96	3/848 (0.4%)
45	DX	0.34	0/635	0.89	2/848 (0.2%)
46	BY	0.43	0/510	0.96	3/677 (0.4%)
46	DY	0.25	0/510	0.69	0/677
47	BZ	0.62	0/453	1.10	3/605 (0.5%)
47	DZ	0.34	0/453	0.82	1/605 (0.2%)
48	B0	0.58	0/450	0.96	0/599
48	D0	0.33	0/450	0.80	0/599
49	B1	0.39	0/417	0.88	0/554
49	D1	0.33	0/417	0.75	0/554
50	B2	0.57	0/380	0.98	2/498 (0.4%)
50	D2	0.34	0/380	0.97	3/498 (0.6%)
51	B3	0.55	0/513	1.04	1/676 (0.1%)
51	D3	0.37	0/513	0.84	1/676 (0.1%)
52	B4	0.54	0/303	1.10	3/397 (0.8%)
52	D4	0.73	2/303 (0.7%)	0.77	0/397
53	CA	0.32	5/36762 (0.0%)	0.96	231/57350 (0.4%)
54	CG	0.30	0/1188	0.86	3/1591 (0.2%)
55	CM	0.26	0/885	0.69	0/1181
56	CP	0.38	0/649	0.82	0/870
57	DA	0.32	1/68314 (0.0%)	0.99	485/106569 (0.5%)
58	DB	0.38	1/2803 (0.0%)	0.96	22/4371 (0.5%)
59	DF	0.31	0/1444	0.83	1/1937 (0.1%)
All	All	0.39	26/306773 (0.0%)	1.00	2037/458565 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	CB	0	1
25	BD	0	1
35	BN	0	1
All	All	0	3

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	CB	146	SER	C-N	20.84	1.57	1.33
2	AB	107	ARG	C-N	20.48	1.60	1.33
58	DB	69	G	O3'-P	-13.44	1.41	1.61
12	CL	21	PRO	C-N	13.25	1.53	1.33
29	DH	48	GLU	C-N	12.92	1.50	1.33

The worst 5 of 2037 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	DB	69	G	O3'-P-O5'	-16.51	79.23	104.00
25	BD	151	THR	CA-C-N	-14.99	103.48	120.12
25	BD	151	THR	C-N-CA	-14.99	103.48	120.12
58	DB	107	G	O3'-P-O5'	-14.40	82.40	104.00
53	CA	1396	A	P-O3'-C3'	12.76	139.33	120.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	BD	9	VAL	Peptide
35	BN	101	GLY	Peptide
2	CB	107	ARG	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32895	0	16553	1465	0
2	AB	1705	0	1732	203	0
2	CB	1705	0	1732	186	0
3	AC	1625	0	1699	130	0
3	CC	1625	0	1699	130	0
4	AD	1643	0	1710	183	0
4	CD	1643	0	1710	189	0
5	AE	1106	0	1148	168	0
5	CE	1106	0	1148	129	0
6	AF	818	0	808	83	0
6	CF	818	0	808	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	AG	1182	0	1240	92	0
8	AH	979	0	1034	114	0
8	CH	979	0	1034	121	0
9	AI	1022	0	1070	96	0
9	CI	1022	0	1070	116	0
10	AJ	787	0	828	84	0
10	CJ	787	0	828	92	0
11	AK	877	0	887	94	0
11	CK	877	0	887	80	0
12	AL	955	0	1019	96	0
12	CL	955	0	1019	106	0
13	AM	884	0	944	73	0
14	AN	774	0	827	86	0
14	CN	769	0	822	88	0
15	AO	714	0	737	66	0
15	CO	714	0	737	62	0
16	AP	649	0	666	64	0
17	AQ	649	0	691	85	0
17	CQ	649	0	691	73	0
18	AR	456	0	478	35	0
18	CR	456	0	478	50	0
19	AS	638	0	665	50	0
19	CS	638	0	665	69	0
20	AT	665	0	714	74	0
20	CT	665	0	714	69	0
21	AU	426	0	449	81	0
21	CU	426	0	449	81	0
22	BA	61274	0	30819	2363	0
23	BB	2529	0	1281	84	0
24	BC	2083	0	2157	237	0
24	DC	2083	0	2157	271	0
25	BD	1565	0	1616	230	0
25	DD	1565	0	1616	205	0
26	BE	1552	0	1619	160	0
26	DE	1552	0	1619	190	0
27	BF	1411	0	1447	145	0
28	BG	1323	0	1374	151	0
28	DG	1323	0	1374	136	0
29	BH	1111	0	1148	115	0
29	DH	1111	0	1148	126	0
30	BI	1032	0	1088	115	0
30	DI	1032	0	1088	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	BJ	1129	0	1162	179	0
31	DJ	1129	0	1162	140	0
32	BK	939	0	1012	114	0
32	DK	939	0	1012	130	0
33	BL	1045	0	1117	126	0
33	DL	1045	0	1117	123	0
34	BM	1074	0	1157	109	0
34	DM	1074	0	1157	115	0
35	BN	961	0	1000	99	0
35	DN	961	0	1000	143	0
36	BO	892	0	923	82	0
36	DO	892	0	923	75	0
37	BP	917	0	965	145	0
37	DP	917	0	965	137	0
38	BQ	947	0	1022	162	0
38	DQ	947	0	1022	130	0
39	BR	816	0	839	119	0
39	DR	816	0	839	87	0
40	BS	857	0	922	87	0
40	DS	857	0	922	84	0
41	BT	739	0	807	118	0
41	DT	739	0	807	111	0
42	BU	780	0	834	55	0
42	DU	780	0	834	93	0
43	BV	753	0	780	75	0
43	DV	753	0	780	75	0
44	BW	596	0	610	212	0
44	DW	596	0	610	121	0
45	BX	625	0	655	71	0
45	DX	625	0	655	89	0
46	BY	509	0	543	50	0
46	DY	509	0	543	67	0
47	BZ	449	0	491	41	0
47	DZ	449	0	491	47	0
48	B0	444	0	461	34	0
48	D0	444	0	461	64	0
49	B1	410	0	440	40	0
49	D1	410	0	440	38	0
50	B2	377	0	418	39	0
50	D2	377	0	418	33	0
51	B3	504	0	574	46	0
51	D3	504	0	574	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	B4	302	0	340	39	0
52	D4	302	0	343	36	0
53	CA	32831	0	16521	1799	0
54	CG	1175	0	1230	133	0
55	CM	877	0	937	102	0
56	CP	639	0	656	75	0
57	DA	60995	0	30679	3812	0
58	DB	2507	0	1270	167	0
59	DF	1420	0	1460	197	0
60	AA	42	0	0	0	0
60	AN	1	0	0	0	0
60	BA	135	0	0	0	0
60	BB	4	0	0	0	0
60	BL	1	0	0	0	0
60	CA	42	0	0	0	0
60	DA	133	0	0	0	0
60	DB	1	0	0	0	0
60	DC	1	0	0	0	0
60	DE	1	0	0	0	0
60	DJ	1	0	0	0	0
61	BA	20	0	11	1	0
62	B4	1	0	0	0	0
62	D4	1	0	0	0	0
63	AA	197	0	0	11	0
63	AL	2	0	0	0	0
63	AN	6	0	0	1	0
63	AT	2	0	0	0	0
63	AU	1	0	0	0	0
63	B2	2	0	0	0	0
63	B3	2	0	0	0	0
63	B4	2	0	0	0	0
63	BA	608	0	0	43	0
63	BB	19	0	0	0	0
63	BC	8	0	0	0	0
63	BD	2	0	0	3	0
63	BE	1	0	0	0	0
63	BL	4	0	0	1	0
63	BN	2	0	0	0	0
63	BQ	1	0	0	0	0
63	BT	2	0	0	1	0
63	BV	1	0	0	1	0
63	CA	195	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	CE	3	0	0	1	0
63	CI	1	0	0	0	0
63	CL	1	0	0	0	0
63	CN	3	0	0	0	0
63	CT	2	0	0	0	0
63	CU	2	0	0	0	0
63	D2	1	0	0	1	0
63	D3	1	0	0	0	0
63	D4	4	0	0	0	0
63	DA	603	0	0	19	0
63	DB	4	0	0	0	0
63	DC	10	0	0	0	0
63	DD	1	0	0	0	0
63	DE	3	0	0	0	0
63	DJ	4	0	0	0	0
63	DL	5	0	0	0	0
63	DN	2	0	0	0	0
63	DT	2	0	0	0	0
63	DU	2	0	0	0	0
63	DV	1	0	0	0	0
All	All	284499	0	190852	18407	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 39.

The worst 5 of 18407 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:DA:2092:U:H1'	57:DA:2093:G:C8	1.52	1.43
38:BQ:63:ARG:NH1	38:BQ:96:ASP:HA	1.44	1.29
57:DA:2092:U:O2'	57:DA:2093:G:H5''	1.08	1.24
38:BQ:63:ARG:HH12	38:BQ:96:ASP:CA	1.55	1.20
28:BG:83:THR:HA	28:BG:84:LYS:NZ	1.57	1.19

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/218 (99%)	132 (61%)	55 (26%)	29 (13%)	0	1
2	CB	216/218 (99%)	149 (69%)	49 (23%)	18 (8%)	0	4
3	AC	204/206 (99%)	153 (75%)	34 (17%)	17 (8%)	0	4
3	CC	204/206 (99%)	145 (71%)	39 (19%)	20 (10%)	0	2
4	AD	203/205 (99%)	133 (66%)	43 (21%)	27 (13%)	0	1
4	CD	203/205 (99%)	138 (68%)	42 (21%)	23 (11%)	0	2
5	AE	148/150 (99%)	103 (70%)	28 (19%)	17 (12%)	0	1
5	CE	148/150 (99%)	106 (72%)	24 (16%)	18 (12%)	0	1
6	AF	98/100 (98%)	71 (72%)	20 (20%)	7 (7%)	1	6
6	CF	98/100 (98%)	68 (69%)	19 (19%)	11 (11%)	0	2
7	AG	149/151 (99%)	108 (72%)	35 (24%)	6 (4%)	2	17
8	AH	127/129 (98%)	94 (74%)	27 (21%)	6 (5%)	2	14
8	CH	127/129 (98%)	89 (70%)	29 (23%)	9 (7%)	1	6
9	AI	125/127 (98%)	84 (67%)	30 (24%)	11 (9%)	0	3
9	CI	125/127 (98%)	90 (72%)	23 (18%)	12 (10%)	0	3
10	AJ	96/98 (98%)	70 (73%)	16 (17%)	10 (10%)	0	2
10	CJ	96/98 (98%)	55 (57%)	26 (27%)	15 (16%)	0	0
11	AK	115/117 (98%)	86 (75%)	20 (17%)	9 (8%)	1	5
11	CK	115/117 (98%)	86 (75%)	20 (17%)	9 (8%)	1	5
12	AL	121/123 (98%)	88 (73%)	16 (13%)	17 (14%)	0	1
12	CL	121/123 (98%)	83 (69%)	30 (25%)	8 (7%)	1	7
13	AM	112/114 (98%)	84 (75%)	19 (17%)	9 (8%)	1	4
14	AN	92/100 (92%)	58 (63%)	22 (24%)	12 (13%)	0	1
14	CN	91/100 (91%)	60 (66%)	26 (29%)	5 (6%)	1	11
15	AO	86/88 (98%)	62 (72%)	13 (15%)	11 (13%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	CO	86/88 (98%)	65 (76%)	18 (21%)	3 (4%)	3	20
16	AP	80/82 (98%)	56 (70%)	15 (19%)	9 (11%)	0	2
17	AQ	78/80 (98%)	55 (70%)	11 (14%)	12 (15%)	0	0
17	CQ	78/80 (98%)	61 (78%)	8 (10%)	9 (12%)	0	1
18	AR	53/55 (96%)	41 (77%)	10 (19%)	2 (4%)	2	18
18	CR	53/55 (96%)	42 (79%)	10 (19%)	1 (2%)	6	33
19	AS	77/79 (98%)	59 (77%)	12 (16%)	6 (8%)	1	5
19	CS	77/79 (98%)	46 (60%)	24 (31%)	7 (9%)	0	3
20	AT	83/85 (98%)	65 (78%)	10 (12%)	8 (10%)	0	3
20	CT	83/85 (98%)	61 (74%)	13 (16%)	9 (11%)	0	2
21	AU	49/51 (96%)	26 (53%)	15 (31%)	8 (16%)	0	0
21	CU	49/51 (96%)	21 (43%)	12 (24%)	16 (33%)	0	0
24	BC	269/271 (99%)	180 (67%)	61 (23%)	28 (10%)	0	2
24	DC	269/271 (99%)	164 (61%)	72 (27%)	33 (12%)	0	1
25	BD	207/209 (99%)	141 (68%)	37 (18%)	29 (14%)	0	1
25	DD	207/209 (99%)	134 (65%)	41 (20%)	32 (16%)	0	0
26	BE	199/201 (99%)	148 (74%)	31 (16%)	20 (10%)	0	2
26	DE	199/201 (99%)	120 (60%)	54 (27%)	25 (13%)	0	1
27	BF	175/177 (99%)	127 (73%)	29 (17%)	19 (11%)	0	2
28	BG	174/176 (99%)	116 (67%)	34 (20%)	24 (14%)	0	1
28	DG	174/176 (99%)	104 (60%)	39 (22%)	31 (18%)	0	0
29	BH	147/149 (99%)	63 (43%)	52 (35%)	32 (22%)	0	0
29	DH	147/149 (99%)	73 (50%)	53 (36%)	21 (14%)	0	1
30	BI	139/141 (99%)	84 (60%)	41 (30%)	14 (10%)	0	2
30	DI	139/141 (99%)	83 (60%)	38 (27%)	18 (13%)	0	1
31	BJ	140/142 (99%)	106 (76%)	20 (14%)	14 (10%)	0	2
31	DJ	140/142 (99%)	92 (66%)	30 (21%)	18 (13%)	0	1
32	BK	120/122 (98%)	83 (69%)	20 (17%)	17 (14%)	0	1
32	DK	120/122 (98%)	77 (64%)	21 (18%)	22 (18%)	0	0
33	BL	141/143 (99%)	95 (67%)	30 (21%)	16 (11%)	0	2
33	DL	141/143 (99%)	78 (55%)	42 (30%)	21 (15%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	BM	134/136 (98%)	96 (72%)	24 (18%)	14 (10%)	0	2
34	DM	134/136 (98%)	94 (70%)	25 (19%)	15 (11%)	0	2
35	BN	118/120 (98%)	88 (75%)	20 (17%)	10 (8%)	0	3
35	DN	118/120 (98%)	67 (57%)	35 (30%)	16 (14%)	0	1
36	BO	114/116 (98%)	88 (77%)	17 (15%)	9 (8%)	1	5
36	DO	114/116 (98%)	79 (69%)	27 (24%)	8 (7%)	1	6
37	BP	112/114 (98%)	74 (66%)	23 (20%)	15 (13%)	0	1
37	DP	112/114 (98%)	66 (59%)	28 (25%)	18 (16%)	0	0
38	BQ	115/117 (98%)	99 (86%)	9 (8%)	7 (6%)	1	9
38	DQ	115/117 (98%)	78 (68%)	24 (21%)	13 (11%)	0	2
39	BR	101/103 (98%)	82 (81%)	11 (11%)	8 (8%)	1	5
39	DR	101/103 (98%)	70 (69%)	21 (21%)	10 (10%)	0	2
40	BS	108/110 (98%)	83 (77%)	16 (15%)	9 (8%)	0	4
40	DS	108/110 (98%)	76 (70%)	24 (22%)	8 (7%)	1	6
41	BT	91/93 (98%)	58 (64%)	20 (22%)	13 (14%)	0	1
41	DT	91/93 (98%)	49 (54%)	26 (29%)	16 (18%)	0	0
42	BU	100/102 (98%)	70 (70%)	16 (16%)	14 (14%)	0	1
42	DU	100/102 (98%)	51 (51%)	27 (27%)	22 (22%)	0	0
43	BV	92/94 (98%)	77 (84%)	14 (15%)	1 (1%)	11	43
43	DV	92/94 (98%)	65 (71%)	22 (24%)	5 (5%)	1	12
44	BW	77/79 (98%)	31 (40%)	18 (23%)	28 (36%)	0	0
44	DW	77/79 (98%)	32 (42%)	26 (34%)	19 (25%)	0	0
45	BX	75/77 (97%)	58 (77%)	13 (17%)	4 (5%)	1	12
45	DX	75/77 (97%)	48 (64%)	19 (25%)	8 (11%)	0	2
46	BY	61/63 (97%)	40 (66%)	13 (21%)	8 (13%)	0	1
46	DY	61/63 (97%)	43 (70%)	13 (21%)	5 (8%)	0	4
47	BZ	56/58 (97%)	43 (77%)	10 (18%)	3 (5%)	1	12
47	DZ	56/58 (97%)	34 (61%)	16 (29%)	6 (11%)	0	2
48	B0	54/56 (96%)	42 (78%)	7 (13%)	5 (9%)	0	3
48	D0	54/56 (96%)	40 (74%)	7 (13%)	7 (13%)	0	1
49	B1	48/50 (96%)	35 (73%)	10 (21%)	3 (6%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	D1	48/50 (96%)	37 (77%)	6 (12%)	5 (10%)	0	2
50	B2	44/46 (96%)	39 (89%)	4 (9%)	1 (2%)	5	29
50	D2	44/46 (96%)	30 (68%)	7 (16%)	7 (16%)	0	0
51	B3	62/64 (97%)	51 (82%)	8 (13%)	3 (5%)	2	14
51	D3	62/64 (97%)	40 (64%)	17 (27%)	5 (8%)	1	4
52	B4	36/38 (95%)	27 (75%)	6 (17%)	3 (8%)	0	4
52	D4	36/38 (95%)	22 (61%)	9 (25%)	5 (14%)	0	1
54	CG	148/150 (99%)	98 (66%)	42 (28%)	8 (5%)	1	12
55	CM	111/113 (98%)	63 (57%)	36 (32%)	12 (11%)	0	2
56	CP	78/80 (98%)	49 (63%)	19 (24%)	10 (13%)	0	1
59	DF	176/178 (99%)	98 (56%)	44 (25%)	34 (19%)	0	0
All	All	11238/11447 (98%)	7571 (67%)	2387 (21%)	1280 (11%)	0	2

5 of 1280 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	20	ARG
2	AB	40	ILE
2	AB	72	LYS
2	AB	75	ALA
2	AB	119	GLN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	180/180 (100%)	144 (80%)	36 (20%)	1	7
2	CB	180/180 (100%)	158 (88%)	22 (12%)	5	22
3	AC	170/170 (100%)	140 (82%)	30 (18%)	2	10
3	CC	170/170 (100%)	154 (91%)	16 (9%)	8	33
4	AD	172/172 (100%)	143 (83%)	29 (17%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	CD	172/172 (100%)	134 (78%)	38 (22%)	1	5
5	AE	113/113 (100%)	84 (74%)	29 (26%)	0	3
5	CE	113/113 (100%)	87 (77%)	26 (23%)	1	5
6	AF	87/87 (100%)	75 (86%)	12 (14%)	3	18
6	CF	87/87 (100%)	75 (86%)	12 (14%)	3	18
7	AG	124/124 (100%)	107 (86%)	17 (14%)	3	18
8	AH	104/104 (100%)	84 (81%)	20 (19%)	1	8
8	CH	104/104 (100%)	88 (85%)	16 (15%)	2	14
9	AI	105/105 (100%)	86 (82%)	19 (18%)	2	9
9	CI	105/105 (100%)	89 (85%)	16 (15%)	3	14
10	AJ	86/86 (100%)	72 (84%)	14 (16%)	2	12
10	CJ	86/86 (100%)	75 (87%)	11 (13%)	4	20
11	AK	90/90 (100%)	76 (84%)	14 (16%)	2	13
11	CK	90/90 (100%)	75 (83%)	15 (17%)	2	11
12	AL	103/103 (100%)	74 (72%)	29 (28%)	0	2
12	CL	103/103 (100%)	83 (81%)	20 (19%)	1	8
13	AM	92/92 (100%)	84 (91%)	8 (9%)	9	36
14	AN	79/83 (95%)	72 (91%)	7 (9%)	9	34
14	CN	79/83 (95%)	70 (89%)	9 (11%)	5	24
15	AO	76/76 (100%)	67 (88%)	9 (12%)	5	23
15	CO	76/76 (100%)	67 (88%)	9 (12%)	5	23
16	AP	65/65 (100%)	53 (82%)	12 (18%)	1	9
17	AQ	74/74 (100%)	57 (77%)	17 (23%)	1	5
17	CQ	74/74 (100%)	60 (81%)	14 (19%)	1	9
18	AR	48/48 (100%)	44 (92%)	4 (8%)	10	38
18	CR	48/48 (100%)	42 (88%)	6 (12%)	4	21
19	AS	70/70 (100%)	60 (86%)	10 (14%)	3	16
19	CS	70/70 (100%)	65 (93%)	5 (7%)	13	44
20	AT	65/65 (100%)	49 (75%)	16 (25%)	1	3
20	CT	65/65 (100%)	54 (83%)	11 (17%)	2	11
21	AU	44/44 (100%)	33 (75%)	11 (25%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	CU	44/44 (100%)	34 (77%)	10 (23%)	1	5
24	BC	216/216 (100%)	168 (78%)	48 (22%)	1	5
24	DC	216/216 (100%)	182 (84%)	34 (16%)	2	13
25	BD	164/164 (100%)	127 (77%)	37 (23%)	1	5
25	DD	164/164 (100%)	132 (80%)	32 (20%)	1	8
26	BE	165/165 (100%)	118 (72%)	47 (28%)	0	2
26	DE	165/165 (100%)	147 (89%)	18 (11%)	6	26
27	BF	148/148 (100%)	118 (80%)	30 (20%)	1	7
28	BG	137/137 (100%)	104 (76%)	33 (24%)	1	4
28	DG	137/137 (100%)	118 (86%)	19 (14%)	3	17
29	BH	114/114 (100%)	93 (82%)	21 (18%)	1	9
29	DH	114/114 (100%)	98 (86%)	16 (14%)	3	17
30	BI	109/109 (100%)	95 (87%)	14 (13%)	4	20
30	DI	109/109 (100%)	102 (94%)	7 (6%)	16	48
31	BJ	116/116 (100%)	86 (74%)	30 (26%)	0	3
31	DJ	116/116 (100%)	95 (82%)	21 (18%)	2	9
32	BK	103/103 (100%)	79 (77%)	24 (23%)	1	5
32	DK	103/103 (100%)	77 (75%)	26 (25%)	0	3
33	BL	102/102 (100%)	70 (69%)	32 (31%)	0	1
33	DL	102/102 (100%)	85 (83%)	17 (17%)	2	11
34	BM	109/109 (100%)	82 (75%)	27 (25%)	1	3
34	DM	109/109 (100%)	88 (81%)	21 (19%)	1	8
35	BN	100/100 (100%)	77 (77%)	23 (23%)	1	5
35	DN	100/100 (100%)	82 (82%)	18 (18%)	2	9
36	BO	86/86 (100%)	66 (77%)	20 (23%)	1	5
36	DO	86/86 (100%)	78 (91%)	8 (9%)	8	33
37	BP	99/99 (100%)	66 (67%)	33 (33%)	0	1
37	DP	99/99 (100%)	90 (91%)	9 (9%)	9	34
38	BQ	89/89 (100%)	71 (80%)	18 (20%)	1	7
38	DQ	89/89 (100%)	71 (80%)	18 (20%)	1	7
39	BR	84/84 (100%)	65 (77%)	19 (23%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	DR	84/84 (100%)	71 (84%)	13 (16%)	2	14
40	BS	93/93 (100%)	69 (74%)	24 (26%)	0	3
40	DS	93/93 (100%)	73 (78%)	20 (22%)	1	6
41	BT	80/80 (100%)	58 (72%)	22 (28%)	0	2
41	DT	80/80 (100%)	73 (91%)	7 (9%)	9	35
42	BU	83/83 (100%)	63 (76%)	20 (24%)	1	4
42	DU	83/83 (100%)	69 (83%)	14 (17%)	2	11
43	BV	78/78 (100%)	59 (76%)	19 (24%)	1	4
43	DV	78/78 (100%)	69 (88%)	9 (12%)	5	24
44	BW	59/59 (100%)	40 (68%)	19 (32%)	0	1
44	DW	59/59 (100%)	46 (78%)	13 (22%)	1	6
45	BX	67/67 (100%)	51 (76%)	16 (24%)	1	4
45	DX	67/67 (100%)	59 (88%)	8 (12%)	5	23
46	BY	55/55 (100%)	41 (74%)	14 (26%)	0	3
46	DY	55/55 (100%)	52 (94%)	3 (6%)	19	52
47	BZ	48/48 (100%)	33 (69%)	15 (31%)	0	1
47	DZ	48/48 (100%)	40 (83%)	8 (17%)	2	11
48	B0	47/47 (100%)	36 (77%)	11 (23%)	1	4
48	D0	47/47 (100%)	40 (85%)	7 (15%)	3	15
49	B1	45/45 (100%)	35 (78%)	10 (22%)	1	5
49	D1	45/45 (100%)	41 (91%)	4 (9%)	9	34
50	B2	38/38 (100%)	30 (79%)	8 (21%)	1	6
50	D2	38/38 (100%)	35 (92%)	3 (8%)	11	40
51	B3	51/51 (100%)	42 (82%)	9 (18%)	2	10
51	D3	51/51 (100%)	40 (78%)	11 (22%)	1	6
52	B4	34/34 (100%)	27 (79%)	7 (21%)	1	7
52	D4	34/34 (100%)	29 (85%)	5 (15%)	3	16
54	CG	123/123 (100%)	99 (80%)	24 (20%)	1	8
55	CM	91/91 (100%)	81 (89%)	10 (11%)	6	26
56	CP	65/65 (100%)	53 (82%)	12 (18%)	1	9
59	DF	149/149 (100%)	121 (81%)	28 (19%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9331/9339 (100%)	7619 (82%)	1712 (18%)	2 9

5 of 1712 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	BY	37	LEU
8	CH	110	MET
39	DR	93	PHE
48	B0	22	THR
46	BY	22	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 356 such sidechains are listed below:

Mol	Chain	Res	Type
12	CL	19	ASN
30	DI	106	GLN
14	CN	65	GLN
24	DC	116	GLN
34	DM	13	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1532/1533 (99%)	511 (33%)	237 (15%)
22	BA	2850/2903 (98%)	908 (31%)	411 (14%)
23	BB	117/118 (99%)	35 (29%)	17 (14%)
53	CA	1529/1530 (99%)	559 (36%)	242 (15%)
57	DA	2838/2904 (97%)	1090 (38%)	504 (17%)
58	DB	116/117 (99%)	39 (33%)	17 (14%)
All	All	8982/9105 (98%)	3142 (34%)	1428 (15%)

5 of 3142 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	6	G
1	AA	7	A
1	AA	8	A
1	AA	9	G

5 of 1428 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
57	DA	87	U
57	DA	1304	A
57	DA	230	G
57	DA	86	G
57	DA	726	G

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 365 ligands modelled in this entry, 364 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
61	CLM	BA	3136	-	20,20,20	2.51	4 (20%)	23,27,27	2.10	7 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	CLM	BA	3136	-	-	3/20/22/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	BA	3136	CLM	O9B-N9	7.58	1.35	1.22
61	BA	3136	CLM	C11-C6	5.51	1.47	1.39
61	BA	3136	CLM	C2-N2	4.16	1.42	1.34
61	BA	3136	CLM	C8-C9	2.61	1.43	1.38

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	BA	3136	CLM	C3-N2-C2	-5.26	114.11	123.25
61	BA	3136	CLM	C6-C5-C3	4.44	119.68	111.72
61	BA	3136	CLM	C4-C3-N2	3.06	114.10	109.28
61	BA	3136	CLM	O4-C4-C3	3.00	118.37	111.10
61	BA	3136	CLM	O5-C5-C3	2.69	115.05	107.90

There are no chirality outliers.

All (3) torsion outliers are listed below:

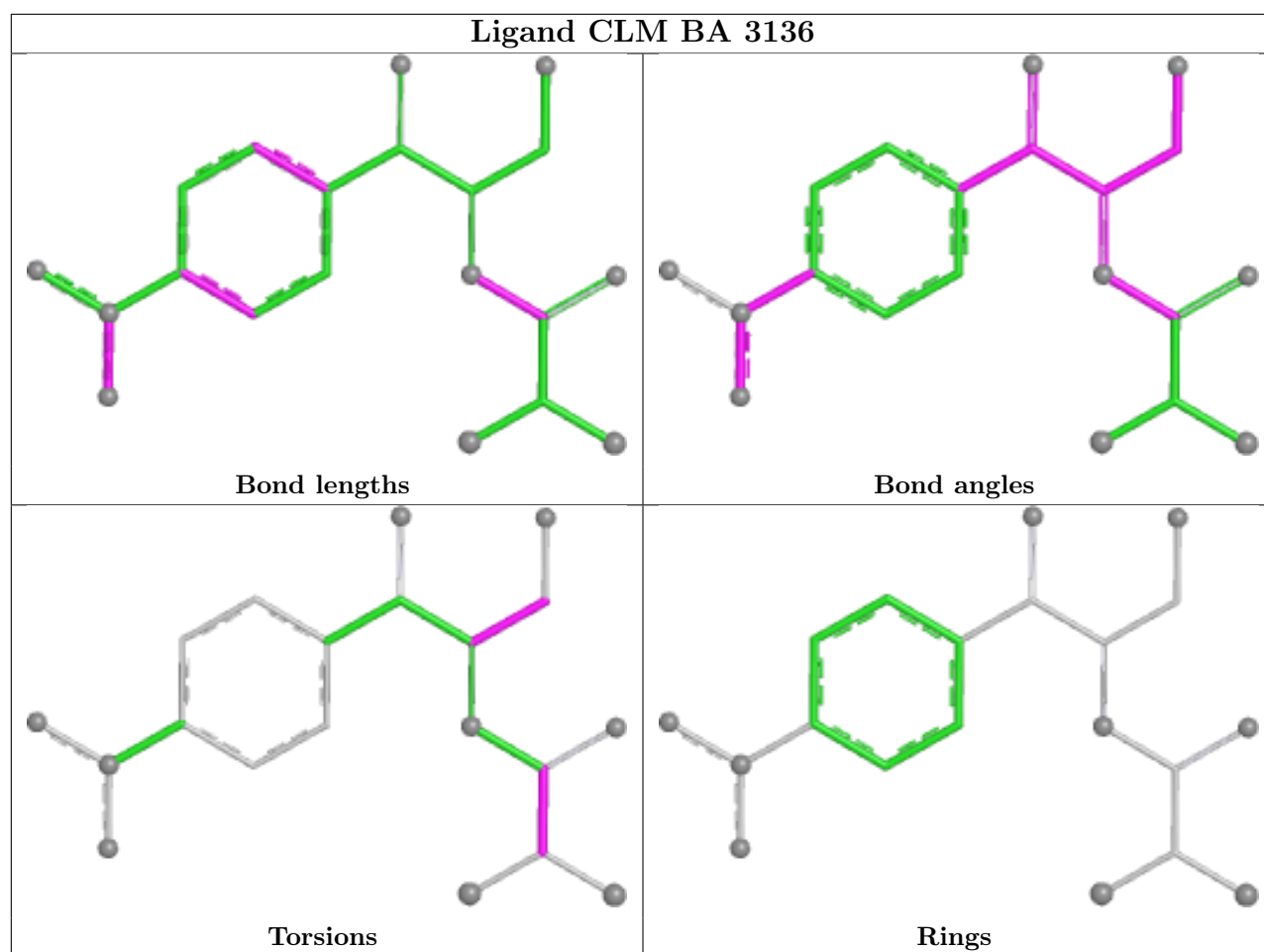
Mol	Chain	Res	Type	Atoms
61	BA	3136	CLM	N2-C3-C4-O4
61	BA	3136	CLM	CL2-C1-C2-N2
61	BA	3136	CLM	CL2-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	BA	3136	CLM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1533/1533 (100%)	-0.41	20 (1%) 75 55	28, 82, 201, 415	0
2	AB	218/218 (100%)	0.63	15 (6%) 23 14	117, 160, 233, 278	0
2	CB	218/218 (100%)	0.95	31 (14%) 6 5	121, 173, 237, 292	0
3	AC	206/206 (100%)	0.16	6 (2%) 53 35	64, 107, 164, 196	0
3	CC	206/206 (100%)	0.73	20 (9%) 13 9	79, 158, 229, 303	0
4	AD	205/205 (100%)	0.32	14 (6%) 23 15	45, 89, 164, 275	0
4	CD	205/205 (100%)	0.35	8 (3%) 43 27	39, 61, 122, 254	0
5	AE	150/150 (100%)	0.32	5 (3%) 49 30	57, 81, 142, 210	0
5	CE	150/150 (100%)	0.89	18 (12%) 9 6	67, 99, 157, 252	0
6	AF	100/100 (100%)	0.42	8 (8%) 18 12	55, 103, 161, 189	0
6	CF	100/100 (100%)	0.61	9 (9%) 15 10	72, 116, 176, 217	0
7	AG	151/151 (100%)	0.58	8 (5%) 32 20	88, 150, 218, 247	0
8	AH	129/129 (100%)	0.05	4 (3%) 51 32	44, 82, 127, 184	0
8	CH	129/129 (100%)	0.74	9 (6%) 22 14	68, 113, 170, 246	0
9	AI	127/127 (100%)	1.34	31 (24%) 2 2	72, 154, 248, 287	0
9	CI	127/127 (100%)	1.63	38 (29%) 1 1	116, 201, 289, 319	0
10	AJ	98/98 (100%)	0.77	14 (14%) 6 5	78, 127, 203, 244	0
10	CJ	98/98 (100%)	1.66	31 (31%) 1 1	114, 204, 278, 301	0
11	AK	117/117 (100%)	0.44	5 (4%) 40 24	47, 117, 196, 238	0
11	CK	117/117 (100%)	0.47	7 (5%) 27 17	68, 117, 175, 239	0
12	AL	123/123 (100%)	0.10	8 (6%) 25 16	24, 57, 121, 180	0
12	CL	123/123 (100%)	0.85	20 (16%) 4 3	44, 89, 144, 226	0
13	AM	114/114 (100%)	0.80	11 (9%) 13 9	90, 158, 240, 281	0
14	AN	96/100 (96%)	1.13	21 (21%) 2 2	76, 122, 214, 271	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
14	CN	95/100 (95%)	1.57	33 (34%)	1 1	123, 239, 369, 399	0
15	AO	88/88 (100%)	0.09	2 (2%)	61 41	40, 81, 123, 187	0
15	CO	88/88 (100%)	0.96	9 (10%)	12 8	76, 122, 190, 265	0
16	AP	82/82 (100%)	0.30	4 (4%)	35 22	46, 79, 155, 228	0
17	AQ	80/80 (100%)	0.44	7 (8%)	15 10	36, 79, 146, 244	0
17	CQ	80/80 (100%)	0.87	10 (12%)	8 6	61, 112, 163, 194	0
18	AR	55/55 (100%)	0.42	3 (5%)	30 19	60, 92, 174, 242	0
18	CR	55/55 (100%)	0.54	6 (10%)	10 7	48, 91, 159, 236	0
19	AS	79/79 (100%)	0.83	11 (13%)	6 5	95, 156, 236, 256	0
19	CS	79/79 (100%)	2.06	33 (41%)	0 1	206, 416, 490, 515	0
20	AT	85/85 (100%)	0.29	7 (8%)	17 11	46, 83, 124, 174	0
20	CT	85/85 (100%)	1.54	25 (29%)	1 1	76, 142, 200, 234	0
21	AU	51/51 (100%)	1.39	13 (25%)	1 2	91, 152, 216, 243	0
21	CU	51/51 (100%)	1.26	14 (27%)	1 1	82, 115, 208, 290	0
22	BA	2854/2903 (98%)	-0.79	47 (1%)	70 51	7, 31, 162, 401	0
23	BB	118/118 (100%)	-0.77	0	100 100	20, 45, 78, 115	0
24	BC	271/271 (100%)	-0.16	5 (1%)	67 48	13, 41, 96, 201	0
24	DC	271/271 (100%)	1.42	66 (24%)	2 2	45, 101, 160, 200	0
25	BD	209/209 (100%)	-0.40	3 (1%)	73 54	7, 29, 80, 144	0
25	DD	209/209 (100%)	1.50	57 (27%)	1 1	60, 123, 193, 270	0
26	BE	201/201 (100%)	-0.25	0	100 100	7, 42, 105, 189	0
26	DE	201/201 (100%)	2.23	101 (50%)	0 1	68, 254, 429, 475	0
27	BF	177/177 (100%)	0.06	4 (2%)	61 41	33, 78, 142, 205	0
28	BG	176/176 (100%)	-0.10	5 (2%)	55 35	23, 62, 124, 215	0
28	DG	176/176 (100%)	1.10	32 (18%)	3 3	79, 207, 297, 363	0
29	BH	149/149 (100%)	1.01	23 (15%)	5 4	41, 178, 274, 301	0
29	DH	149/149 (100%)	1.56	48 (32%)	1 1	93, 182, 270, 305	0
30	BI	141/141 (100%)	1.55	42 (29%)	1 1	171, 257, 316, 355	0
30	DI	141/141 (100%)	1.48	36 (25%)	1 2	227, 344, 382, 400	0
31	BJ	142/142 (100%)	-0.30	3 (2%)	63 43	9, 23, 68, 127	0
31	DJ	142/142 (100%)	1.17	29 (20%)	3 2	63, 122, 184, 223	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
32	BK	122/122 (100%)	-0.43	1 (0%) 82 67	14, 31, 84, 254	0
32	DK	122/122 (100%)	0.84	10 (8%) 17 11	57, 106, 172, 204	0
33	BL	143/143 (100%)	-0.20	1 (0%) 84 69	9, 37, 80, 126	0
33	DL	143/143 (100%)	2.26	72 (50%) 0 1	68, 176, 296, 329	0
34	BM	136/136 (100%)	-0.52	1 (0%) 84 69	9, 29, 71, 133	0
34	DM	136/136 (100%)	1.00	22 (16%) 4 3	47, 126, 187, 223	0
35	BN	120/120 (100%)	-0.49	0 100 100	10, 25, 48, 123	0
35	DN	120/120 (100%)	2.15	56 (46%) 0 1	90, 149, 231, 305	0
36	BO	116/116 (100%)	-0.09	2 (1%) 69 49	28, 49, 93, 126	0
36	DO	116/116 (100%)	0.97	14 (12%) 8 6	132, 176, 238, 280	0
37	BP	114/114 (100%)	-0.36	3 (2%) 57 37	17, 39, 95, 184	0
37	DP	114/114 (100%)	1.13	18 (15%) 5 4	63, 122, 187, 204	0
38	BQ	117/117 (100%)	-0.46	0 100 100	7, 20, 46, 100	0
38	DQ	117/117 (100%)	1.99	53 (45%) 0 1	78, 127, 221, 298	0
39	BR	103/103 (100%)	-0.33	1 (0%) 79 63	7, 34, 78, 139	0
39	DR	103/103 (100%)	1.95	39 (37%) 1 1	80, 157, 275, 306	0
40	BS	110/110 (100%)	-0.54	0 100 100	8, 23, 56, 172	0
40	DS	110/110 (100%)	2.10	49 (44%) 0 1	69, 142, 254, 323	0
41	BT	93/93 (100%)	0.43	6 (6%) 25 16	22, 53, 135, 194	0
41	DT	93/93 (100%)	3.22	71 (76%) 0 0	125, 241, 359, 398	0
42	BU	102/102 (100%)	0.08	2 (1%) 65 45	22, 54, 111, 237	0
42	DU	102/102 (100%)	3.04	71 (69%) 0 0	135, 334, 460, 561	0
43	BV	94/94 (100%)	-0.27	0 100 100	18, 47, 89, 149	0
43	DV	94/94 (100%)	0.71	6 (6%) 25 16	109, 156, 208, 233	0
44	BW	79/79 (100%)	0.29	7 (8%) 15 10	13, 36, 90, 194	0
44	DW	79/79 (100%)	2.30	42 (53%) 0 1	99, 166, 250, 315	0
45	BX	77/77 (100%)	-0.26	0 100 100	17, 42, 87, 113	0
45	DX	77/77 (100%)	2.10	34 (44%) 0 1	72, 122, 190, 222	0
46	BY	63/63 (100%)	0.48	4 (6%) 26 17	34, 73, 121, 155	0
46	DY	63/63 (100%)	3.05	45 (71%) 0 0	159, 374, 464, 494	0
47	BZ	58/58 (100%)	-0.44	0 100 100	7, 26, 61, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
47	DZ	58/58 (100%)	1.27	13 (22%) 2 2	80, 142, 228, 257	0
48	B0	56/56 (100%)	-0.49	0 100 100	6, 26, 80, 127	0
48	D0	56/56 (100%)	1.80	20 (35%) 1 1	75, 148, 244, 284	0
49	B1	50/50 (100%)	0.01	0 100 100	42, 66, 121, 173	0
49	D1	50/50 (100%)	1.54	14 (28%) 1 1	114, 179, 216, 264	0
50	B2	46/46 (100%)	-0.33	1 (2%) 62 42	11, 27, 56, 164	0
50	D2	46/46 (100%)	2.45	27 (58%) 0 0	79, 130, 179, 205	0
51	B3	64/64 (100%)	-0.44	0 100 100	11, 29, 53, 81	0
51	D3	64/64 (100%)	3.29	46 (71%) 0 0	85, 145, 232, 281	0
52	B4	38/38 (100%)	0.12	0 100 100	29, 53, 95, 103	0
52	D4	38/38 (100%)	3.29	31 (81%) 0 0	87, 165, 229, 248	0
53	CA	1530/1530 (100%)	0.53	89 (5%) 29 18	43, 110, 301, 420	0
54	CG	150/150 (100%)	1.41	28 (18%) 3 2	101, 233, 303, 344	0
55	CM	113/113 (100%)	2.67	69 (61%) 0 0	226, 447, 522, 562	0
56	CP	80/80 (100%)	0.90	9 (11%) 10 7	49, 105, 165, 226	0
57	DA	2841/2904 (97%)	1.09	474 (16%) 4 3	51, 132, 279, 491	0
58	DB	117/117 (100%)	0.63	6 (5%) 33 21	107, 180, 240, 264	0
59	DF	178/178 (100%)	0.81	13 (7%) 21 13	175, 239, 286, 345	0
All	All	20431/20552 (99%)	0.50	2509 (12%) 8 6	6, 103, 285, 562	0

The worst 5 of 2509 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
55	CM	97	ARG	13.3
42	DU	30	SER	12.7
51	D3	50	SER	10.1
55	CM	98	GLY	10.0
37	DP	109	ILE	9.2

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
60	MG	DA	3057	1/1	0.05	0.26	257,257,257,257	0
60	MG	DA	3019	1/1	0.35	0.27	252,252,252,252	0
60	MG	CA	1615	1/1	0.40	0.14	243,243,243,243	0
60	MG	DA	3003	1/1	0.49	0.30	253,253,253,253	0
60	MG	CA	1616	1/1	0.53	0.17	279,279,279,279	0
60	MG	DA	3124	1/1	0.53	0.47	211,211,211,211	0
60	MG	AA	1629	1/1	0.60	0.12	227,227,227,227	0
60	MG	DA	3002	1/1	0.60	0.28	229,229,229,229	0
60	MG	DA	3041	1/1	0.62	0.16	133,133,133,133	0
60	MG	DJ	201	1/1	0.63	0.30	331,331,331,331	0
60	MG	DA	3017	1/1	0.64	0.18	147,147,147,147	0
60	MG	DA	3130	1/1	0.65	0.23	305,305,305,305	0
60	MG	BA	3068	1/1	0.67	0.13	174,174,174,174	0
60	MG	DA	3015	1/1	0.68	0.17	277,277,277,277	0
60	MG	DA	3013	1/1	0.68	0.23	209,209,209,209	0
60	MG	DA	3040	1/1	0.69	0.11	120,120,120,120	0
60	MG	DA	3061	1/1	0.70	0.29	210,210,210,210	0
60	MG	BA	3111	1/1	0.72	0.17	93,93,93,93	0
60	MG	CA	1634	1/1	0.72	0.11	200,200,200,200	0
60	MG	DA	3073	1/1	0.72	0.46	276,276,276,276	0
60	MG	DA	3027	1/1	0.73	0.29	277,277,277,277	0
60	MG	CA	1618	1/1	0.73	0.15	141,141,141,141	0
60	MG	DE	301	1/1	0.73	0.24	191,191,191,191	0
60	MG	CA	1602	1/1	0.73	0.18	131,131,131,131	0
60	MG	CA	1627	1/1	0.74	0.17	220,220,220,220	0
60	MG	CA	1612	1/1	0.74	0.22	133,133,133,133	0
60	MG	BA	3024	1/1	0.74	0.28	206,206,206,206	0
60	MG	DA	3024	1/1	0.75	0.18	147,147,147,147	0
60	MG	DA	3032	1/1	0.76	0.21	193,193,193,193	0
60	MG	DA	3007	1/1	0.77	0.16	188,188,188,188	0
60	MG	DC	301	1/1	0.77	0.21	134,134,134,134	0
60	MG	DA	3018	1/1	0.78	0.15	225,225,225,225	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
60	MG	DA	3062	1/1	0.78	0.65	262,262,262,262	0
60	MG	DA	3048	1/1	0.78	0.09	243,243,243,243	0
60	MG	DA	3005	1/1	0.78	0.17	280,280,280,280	0
60	MG	DA	3108	1/1	0.79	0.16	123,123,123,123	0
60	MG	DA	3044	1/1	0.80	0.14	230,230,230,230	0
60	MG	CA	1629	1/1	0.80	0.11	214,214,214,214	0
60	MG	DA	3042	1/1	0.81	0.12	166,166,166,166	0
60	MG	DA	3052	1/1	0.81	0.13	105,105,105,105	0
60	MG	CA	1622	1/1	0.82	0.11	196,196,196,196	0
60	MG	BA	3130	1/1	0.82	0.34	257,257,257,257	0
60	MG	DA	3133	1/1	0.82	0.14	241,241,241,241	0
60	MG	CA	1628	1/1	0.82	0.14	259,259,259,259	0
60	MG	AN	201	1/1	0.82	0.19	219,219,219,219	0
60	MG	DA	3109	1/1	0.82	0.11	169,169,169,169	0
60	MG	DA	3110	1/1	0.83	0.10	174,174,174,174	0
60	MG	DA	3112	1/1	0.83	0.11	114,114,114,114	0
60	MG	DA	3063	1/1	0.83	0.24	305,305,305,305	0
60	MG	DA	3077	1/1	0.83	0.21	259,259,259,259	0
60	MG	AA	1610	1/1	0.84	0.11	200,200,200,200	0
60	MG	DA	3083	1/1	0.84	0.11	176,176,176,176	0
60	MG	DA	3085	1/1	0.84	0.16	127,127,127,127	0
60	MG	DA	3090	1/1	0.84	0.35	209,209,209,209	0
60	MG	DA	3105	1/1	0.84	0.29	305,305,305,305	0
60	MG	DA	3107	1/1	0.84	0.23	201,201,201,201	0
60	MG	DA	3025	1/1	0.84	0.38	253,253,253,253	0
60	MG	CA	1611	1/1	0.84	0.11	116,116,116,116	0
60	MG	DA	3011	1/1	0.85	0.18	215,215,215,215	0
60	MG	DA	3093	1/1	0.85	0.24	166,166,166,166	0
60	MG	DA	3037	1/1	0.85	0.13	203,203,203,203	0
60	MG	DA	3079	1/1	0.85	0.13	149,149,149,149	0
60	MG	DA	3082	1/1	0.85	0.12	214,214,214,214	0
60	MG	DA	3030	1/1	0.85	0.10	66,66,66,66	0
60	MG	DA	3068	1/1	0.85	0.21	225,225,225,225	0
60	MG	DA	3021	1/1	0.86	0.13	169,169,169,169	0
60	MG	CA	1617	1/1	0.86	0.12	205,205,205,205	0
60	MG	CA	1640	1/1	0.86	0.22	171,171,171,171	0
60	MG	DA	3074	1/1	0.86	0.24	239,239,239,239	0
60	MG	DA	3075	1/1	0.86	0.29	229,229,229,229	0
60	MG	AA	1614	1/1	0.86	0.33	201,201,201,201	0
60	MG	DA	3114	1/1	0.87	0.20	166,166,166,166	0
60	MG	DA	3117	1/1	0.87	0.10	99,99,99,99	0
60	MG	CA	1632	1/1	0.87	0.10	143,143,143,143	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	CA	1614	1/1	0.87	0.28	271,271,271,271	0
60	MG	DA	3132	1/1	0.87	0.20	225,225,225,225	0
60	MG	DA	3038	1/1	0.87	0.12	163,163,163,163	0
60	MG	DA	3091	1/1	0.87	0.17	167,167,167,167	0
60	MG	CA	1619	1/1	0.87	0.11	243,243,243,243	0
60	MG	DA	3094	1/1	0.87	0.11	98,98,98,98	0
60	MG	DA	3087	1/1	0.88	0.09	178,178,178,178	0
60	MG	CA	1639	1/1	0.88	0.07	148,148,148,148	0
60	MG	AA	1618	1/1	0.88	0.23	217,217,217,217	0
60	MG	DA	3122	1/1	0.88	0.13	155,155,155,155	0
60	MG	CA	1603	1/1	0.88	0.13	140,140,140,140	0
60	MG	DA	3127	1/1	0.88	0.53	274,274,274,274	0
60	MG	CA	1630	1/1	0.88	0.12	176,176,176,176	0
60	MG	BA	3110	1/1	0.88	0.09	65,65,65,65	0
60	MG	DA	3081	1/1	0.88	0.17	143,143,143,143	0
60	MG	BB	201	1/1	0.88	0.13	246,246,246,246	0
60	MG	DA	3046	1/1	0.88	0.13	152,152,152,152	0
60	MG	DA	3071	1/1	0.88	0.10	136,136,136,136	0
60	MG	CA	1636	1/1	0.89	0.13	130,130,130,130	0
60	MG	DA	3049	1/1	0.89	0.12	150,150,150,150	0
60	MG	DA	3008	1/1	0.89	0.14	153,153,153,153	0
60	MG	DA	3072	1/1	0.89	0.05	193,193,193,193	0
60	MG	DB	201	1/1	0.89	0.12	109,109,109,109	0
60	MG	DA	3035	1/1	0.89	0.17	228,228,228,228	0
60	MG	CA	1610	1/1	0.89	0.13	220,220,220,220	0
60	MG	BA	3123	1/1	0.89	0.32	112,112,112,112	0
60	MG	BA	3134	1/1	0.90	0.27	145,145,145,145	0
60	MG	BA	3035	1/1	0.90	0.25	241,241,241,241	0
60	MG	DA	3128	1/1	0.90	0.20	138,138,138,138	0
60	MG	DA	3092	1/1	0.90	0.11	209,209,209,209	0
60	MG	CA	1601	1/1	0.90	0.11	123,123,123,123	0
60	MG	BA	3109	1/1	0.90	0.12	105,105,105,105	0
60	MG	DA	3096	1/1	0.90	0.19	180,180,180,180	0
60	MG	DA	3100	1/1	0.90	0.21	149,149,149,149	0
60	MG	DA	3121	1/1	0.90	0.10	114,114,114,114	0
60	MG	DA	3001	1/1	0.90	0.15	149,149,149,149	0
60	MG	AA	1630	1/1	0.91	0.13	209,209,209,209	0
60	MG	DA	3006	1/1	0.91	0.11	149,149,149,149	0
60	MG	CA	1620	1/1	0.91	0.15	209,209,209,209	0
60	MG	AA	1638	1/1	0.91	0.09	139,139,139,139	0
60	MG	DA	3010	1/1	0.91	0.29	261,261,261,261	0
60	MG	DA	3099	1/1	0.91	0.14	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	1627	1/1	0.91	0.19	165,165,165,165	0
60	MG	AA	1626	1/1	0.91	0.13	185,185,185,185	0
60	MG	DA	3026	1/1	0.91	0.12	139,139,139,139	0
60	MG	DA	3067	1/1	0.92	0.09	95,95,95,95	0
60	MG	CA	1625	1/1	0.92	0.11	160,160,160,160	0
60	MG	AA	1604	1/1	0.92	0.10	112,112,112,112	0
60	MG	DA	3034	1/1	0.92	0.21	156,156,156,156	0
60	MG	BA	3132	1/1	0.92	0.19	145,145,145,145	0
60	MG	AA	1617	1/1	0.92	0.08	111,111,111,111	0
60	MG	BA	3086	1/1	0.92	0.16	144,144,144,144	0
60	MG	BA	3114	1/1	0.92	0.10	148,148,148,148	0
60	MG	BA	3091	1/1	0.92	0.18	131,131,131,131	0
60	MG	DA	3016	1/1	0.92	0.09	75,75,75,75	0
60	MG	DA	3098	1/1	0.92	0.09	218,218,218,218	0
60	MG	BA	3060	1/1	0.93	0.20	257,257,257,257	0
60	MG	DA	3023	1/1	0.93	0.08	90,90,90,90	0
60	MG	DA	3126	1/1	0.93	0.10	129,129,129,129	0
60	MG	DA	3106	1/1	0.93	0.07	55,55,55,55	0
60	MG	DA	3014	1/1	0.93	0.21	177,177,177,177	0
60	MG	DA	3056	1/1	0.93	0.39	243,243,243,243	0
60	MG	CA	1607	1/1	0.93	0.09	222,222,222,222	0
60	MG	BA	3027	1/1	0.93	0.06	34,34,34,34	0
60	MG	CA	1631	1/1	0.93	0.10	111,111,111,111	0
60	MG	DA	3029	1/1	0.93	0.16	135,135,135,135	0
60	MG	BA	3082	1/1	0.93	0.10	98,98,98,98	0
60	MG	AA	1622	1/1	0.93	0.06	185,185,185,185	0
60	MG	CA	1637	1/1	0.94	0.15	140,140,140,140	0
60	MG	BA	3059	1/1	0.94	0.17	147,147,147,147	0
60	MG	CA	1608	1/1	0.94	0.17	82,82,82,82	0
60	MG	BA	3004	1/1	0.94	0.10	150,150,150,150	0
60	MG	DA	3097	1/1	0.94	0.14	143,143,143,143	0
60	MG	DA	3125	1/1	0.94	0.08	132,132,132,132	0
60	MG	AA	1635	1/1	0.94	0.10	198,198,198,198	0
60	MG	BA	3069	1/1	0.94	0.13	223,223,223,223	0
60	MG	DA	3059	1/1	0.94	0.30	241,241,241,241	0
60	MG	BA	3075	1/1	0.94	0.09	74,74,74,74	0
60	MG	DA	3131	1/1	0.94	0.09	104,104,104,104	0
60	MG	AA	1619	1/1	0.94	0.06	165,165,165,165	0
60	MG	BA	3033	1/1	0.94	0.15	89,89,89,89	0
60	MG	DA	3086	1/1	0.94	0.09	185,185,185,185	0
60	MG	AA	1612	1/1	0.94	0.08	103,103,103,103	0
60	MG	BA	3046	1/1	0.94	0.09	142,142,142,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	3058	1/1	0.94	0.13	106,106,106,106	0
60	MG	CA	1633	1/1	0.95	0.06	82,82,82,82	0
60	MG	DA	3028	1/1	0.95	0.36	195,195,195,195	0
60	MG	DA	3070	1/1	0.95	0.10	61,61,61,61	0
60	MG	DA	3119	1/1	0.95	0.12	84,84,84,84	0
60	MG	BA	3044	1/1	0.95	0.09	56,56,56,56	0
60	MG	DA	3047	1/1	0.95	0.08	82,82,82,82	0
60	MG	AA	1623	1/1	0.95	0.07	104,104,104,104	0
60	MG	BA	3087	1/1	0.95	0.10	182,182,182,182	0
60	MG	BA	3090	1/1	0.95	0.10	93,93,93,93	0
60	MG	DA	3076	1/1	0.95	0.06	110,110,110,110	0
60	MG	DA	3055	1/1	0.95	0.10	121,121,121,121	0
60	MG	DA	3129	1/1	0.95	0.27	271,271,271,271	0
60	MG	AA	1636	1/1	0.95	0.10	149,149,149,149	0
60	MG	DA	3102	1/1	0.95	0.13	105,105,105,105	0
60	MG	DA	3080	1/1	0.95	0.12	70,70,70,70	0
60	MG	DA	3036	1/1	0.95	0.11	111,111,111,111	0
60	MG	CA	1641	1/1	0.95	0.10	73,73,73,73	0
60	MG	DA	3012	1/1	0.95	0.06	57,57,57,57	0
60	MG	BA	3026	1/1	0.95	0.12	122,122,122,122	0
60	MG	CA	1623	1/1	0.95	0.09	79,79,79,79	0
62	ZN	B4	101	1/1	0.95	0.08	81,81,81,81	0
60	MG	DA	3050	1/1	0.96	0.07	89,89,89,89	0
60	MG	DA	3095	1/1	0.96	0.14	110,110,110,110	0
60	MG	AA	1632	1/1	0.96	0.07	53,53,53,53	0
60	MG	BA	3003	1/1	0.96	0.06	44,44,44,44	0
60	MG	AA	1608	1/1	0.96	0.07	38,38,38,38	0
60	MG	BA	3089	1/1	0.96	0.04	39,39,39,39	0
60	MG	CA	1606	1/1	0.96	0.07	77,77,77,77	0
60	MG	DA	3101	1/1	0.96	0.07	73,73,73,73	0
60	MG	DA	3060	1/1	0.96	0.10	144,144,144,144	0
60	MG	DA	3103	1/1	0.96	0.07	36,36,36,36	0
60	MG	DA	3022	1/1	0.96	0.08	118,118,118,118	0
60	MG	BA	3047	1/1	0.96	0.11	112,112,112,112	0
60	MG	CA	1635	1/1	0.96	0.06	85,85,85,85	0
60	MG	DA	3064	1/1	0.96	0.06	65,65,65,65	0
60	MG	BA	3054	1/1	0.96	0.14	214,214,214,214	0
60	MG	BA	3097	1/1	0.96	0.17	182,182,182,182	0
60	MG	BA	3098	1/1	0.96	0.08	46,46,46,46	0
60	MG	BA	3104	1/1	0.96	0.09	27,27,27,27	0
60	MG	CA	1613	1/1	0.96	0.06	116,116,116,116	0
60	MG	CA	1642	1/1	0.96	0.07	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	3055	1/1	0.96	0.21	240,240,240,240	0
60	MG	BA	3056	1/1	0.96	0.11	86,86,86,86	0
60	MG	BA	3010	1/1	0.96	0.06	48,48,48,48	0
60	MG	BA	3022	1/1	0.96	0.07	20,20,20,20	0
60	MG	BA	3115	1/1	0.96	0.10	8,8,8,8	0
60	MG	BA	3117	1/1	0.96	0.07	79,79,79,79	0
60	MG	DA	3039	1/1	0.96	0.05	59,59,59,59	0
60	MG	AA	1607	1/1	0.96	0.07	98,98,98,98	0
60	MG	DA	3009	1/1	0.96	0.07	75,75,75,75	0
60	MG	DA	3084	1/1	0.96	0.10	157,157,157,157	0
60	MG	AA	1616	1/1	0.96	0.10	123,123,123,123	0
60	MG	BA	3131	1/1	0.96	0.09	96,96,96,96	0
60	MG	DA	3045	1/1	0.96	0.07	76,76,76,76	0
60	MG	CA	1624	1/1	0.96	0.09	123,123,123,123	0
60	MG	AA	1639	1/1	0.96	0.06	92,92,92,92	0
60	MG	AA	1640	1/1	0.96	0.12	189,189,189,189	0
60	MG	BA	3135	1/1	0.96	0.26	204,204,204,204	0
62	ZN	D4	101	1/1	0.96	0.07	197,197,197,197	0
60	MG	AA	1603	1/1	0.97	0.07	131,131,131,131	0
60	MG	DA	3058	1/1	0.97	0.17	204,204,204,204	0
60	MG	DA	3111	1/1	0.97	0.09	89,89,89,89	0
60	MG	CA	1638	1/1	0.97	0.06	106,106,106,106	0
60	MG	DA	3113	1/1	0.97	0.08	123,123,123,123	0
60	MG	BA	3011	1/1	0.97	0.12	149,149,149,149	0
60	MG	DA	3115	1/1	0.97	0.12	69,69,69,69	0
60	MG	DA	3116	1/1	0.97	0.05	59,59,59,59	0
60	MG	BA	3014	1/1	0.97	0.08	75,75,75,75	0
60	MG	CA	1604	1/1	0.97	0.05	65,65,65,65	0
60	MG	DA	3120	1/1	0.97	0.10	84,84,84,84	0
60	MG	AA	1601	1/1	0.97	0.07	93,93,93,93	0
60	MG	AA	1620	1/1	0.97	0.07	120,120,120,120	0
60	MG	BA	3002	1/1	0.97	0.07	60,60,60,60	0
60	MG	BA	3118	1/1	0.97	0.15	136,136,136,136	0
60	MG	DA	3069	1/1	0.97	0.06	93,93,93,93	0
60	MG	DA	3043	1/1	0.97	0.15	112,112,112,112	0
60	MG	DA	3004	1/1	0.97	0.11	86,86,86,86	0
60	MG	AA	1628	1/1	0.97	0.04	70,70,70,70	0
60	MG	BA	3124	1/1	0.97	0.07	22,22,22,22	0
60	MG	BA	3092	1/1	0.97	0.05	30,30,30,30	0
60	MG	BA	3094	1/1	0.97	0.07	42,42,42,42	0
60	MG	BA	3096	1/1	0.97	0.08	59,59,59,59	0
60	MG	AA	1602	1/1	0.97	0.05	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	DA	3104	1/1	0.97	0.07	48,48,48,48	0
60	MG	BA	3005	1/1	0.97	0.05	60,60,60,60	0
60	MG	DA	3054	1/1	0.97	0.09	125,125,125,125	0
61	CLM	BA	3136	20/20	0.97	0.09	2,26,77,92	0
60	MG	DA	3031	1/1	0.97	0.07	121,121,121,121	0
60	MG	BA	3008	1/1	0.97	0.09	29,29,29,29	0
60	MG	AA	1637	1/1	0.98	0.05	34,34,34,34	0
60	MG	AA	1631	1/1	0.98	0.07	95,95,95,95	0
60	MG	BA	3100	1/1	0.98	0.06	26,26,26,26	0
60	MG	CA	1605	1/1	0.98	0.09	47,47,47,47	0
60	MG	BA	3073	1/1	0.98	0.08	116,116,116,116	0
60	MG	DA	3078	1/1	0.98	0.05	95,95,95,95	0
60	MG	BA	3107	1/1	0.98	0.08	8,8,8,8	0
60	MG	BA	3045	1/1	0.98	0.05	13,13,13,13	0
60	MG	BA	3077	1/1	0.98	0.07	151,151,151,151	0
60	MG	BA	3078	1/1	0.98	0.05	49,49,49,49	0
60	MG	DA	3051	1/1	0.98	0.04	49,49,49,49	0
60	MG	BA	3079	1/1	0.98	0.04	20,20,20,20	0
60	MG	DA	3118	1/1	0.98	0.07	75,75,75,75	0
60	MG	DA	3053	1/1	0.98	0.04	78,78,78,78	0
60	MG	BA	3081	1/1	0.98	0.08	41,41,41,41	0
60	MG	BA	3015	1/1	0.98	0.14	30,30,30,30	0
60	MG	DA	3088	1/1	0.98	0.08	102,102,102,102	0
60	MG	DA	3123	1/1	0.98	0.07	65,65,65,65	0
60	MG	DA	3089	1/1	0.98	0.05	81,81,81,81	0
60	MG	BA	3083	1/1	0.98	0.06	52,52,52,52	0
60	MG	BA	3122	1/1	0.98	0.07	25,25,25,25	0
60	MG	AA	1624	1/1	0.98	0.09	139,139,139,139	0
60	MG	BA	3049	1/1	0.98	0.05	72,72,72,72	0
60	MG	BA	3125	1/1	0.98	0.04	26,26,26,26	0
60	MG	AA	1606	1/1	0.98	0.05	58,58,58,58	0
60	MG	DA	3033	1/1	0.98	0.11	91,91,91,91	0
60	MG	CA	1621	1/1	0.98	0.15	60,60,60,60	0
60	MG	BA	3025	1/1	0.98	0.11	38,38,38,38	0
60	MG	DA	3065	1/1	0.98	0.04	40,40,40,40	0
60	MG	BA	3007	1/1	0.98	0.07	84,84,84,84	0
60	MG	AA	1609	1/1	0.98	0.04	47,47,47,47	0
60	MG	BA	3028	1/1	0.98	0.11	45,45,45,45	0
60	MG	BA	3095	1/1	0.98	0.01	13,13,13,13	0
60	MG	BB	202	1/1	0.98	0.05	54,54,54,54	0
60	MG	BA	3001	1/1	0.98	0.06	84,84,84,84	0
60	MG	BA	3127	1/1	0.99	0.04	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	3080	1/1	0.99	0.04	25,25,25,25	0
60	MG	BA	3042	1/1	0.99	0.05	34,34,34,34	0
60	MG	AA	1633	1/1	0.99	0.04	52,52,52,52	0
60	MG	AA	1634	1/1	0.99	0.03	58,58,58,58	0
60	MG	BA	3085	1/1	0.99	0.04	24,24,24,24	0
60	MG	AA	1621	1/1	0.99	0.10	35,35,35,35	0
60	MG	BA	3017	1/1	0.99	0.02	27,27,27,27	0
60	MG	BB	203	1/1	0.99	0.04	16,16,16,16	0
60	MG	BB	204	1/1	0.99	0.04	30,30,30,30	0
60	MG	BL	201	1/1	0.99	0.04	34,34,34,34	0
60	MG	BA	3088	1/1	0.99	0.04	22,22,22,22	0
60	MG	AA	1613	1/1	0.99	0.04	56,56,56,56	0
60	MG	BA	3050	1/1	0.99	0.03	12,12,12,12	0
60	MG	BA	3051	1/1	0.99	0.05	48,48,48,48	0
60	MG	BA	3052	1/1	0.99	0.03	12,12,12,12	0
60	MG	BA	3093	1/1	0.99	0.06	68,68,68,68	0
60	MG	AA	1611	1/1	0.99	0.05	81,81,81,81	0
60	MG	AA	1615	1/1	0.99	0.03	127,127,127,127	0
60	MG	CA	1609	1/1	0.99	0.04	71,71,71,71	0
60	MG	BA	3006	1/1	0.99	0.03	47,47,47,47	0
60	MG	BA	3057	1/1	0.99	0.04	43,43,43,43	0
60	MG	AA	1625	1/1	0.99	0.14	31,31,31,31	0
60	MG	DA	3066	1/1	0.99	0.04	65,65,65,65	0
60	MG	AA	1605	1/1	0.99	0.04	30,30,30,30	0
60	MG	BA	3101	1/1	0.99	0.09	105,105,105,105	0
60	MG	DA	3020	1/1	0.99	0.11	36,36,36,36	0
60	MG	BA	3103	1/1	0.99	0.08	8,8,8,8	0
60	MG	BA	3029	1/1	0.99	0.09	10,10,10,10	0
60	MG	BA	3106	1/1	0.99	0.05	13,13,13,13	0
60	MG	BA	3061	1/1	0.99	0.03	11,11,11,11	0
60	MG	BA	3108	1/1	0.99	0.06	6,6,6,6	0
60	MG	BA	3067	1/1	0.99	0.03	22,22,22,22	0
60	MG	BA	3030	1/1	0.99	0.05	34,34,34,34	0
60	MG	BA	3031	1/1	0.99	0.04	15,15,15,15	0
60	MG	BA	3112	1/1	0.99	0.07	33,33,33,33	0
60	MG	BA	3113	1/1	0.99	0.04	34,34,34,34	0
60	MG	BA	3070	1/1	0.99	0.06	76,76,76,76	0
60	MG	CA	1626	1/1	0.99	0.11	27,27,27,27	0
60	MG	BA	3072	1/1	0.99	0.07	81,81,81,81	0
60	MG	BA	3009	1/1	0.99	0.05	12,12,12,12	0
60	MG	BA	3034	1/1	0.99	0.02	9,9,9,9	0
60	MG	BA	3119	1/1	0.99	0.05	15,15,15,15	0

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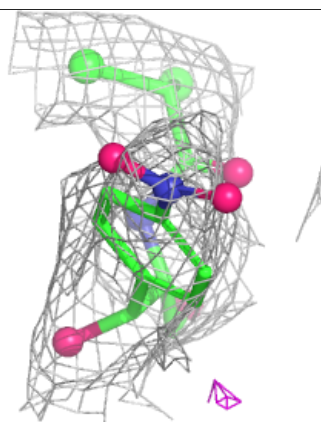
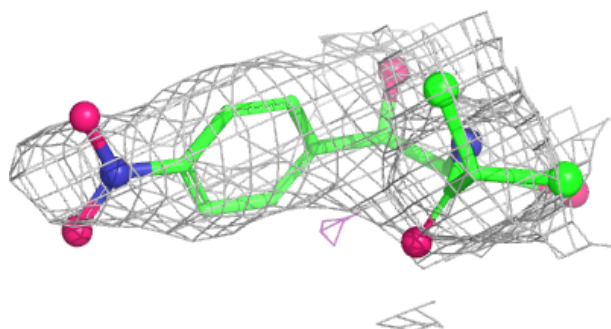
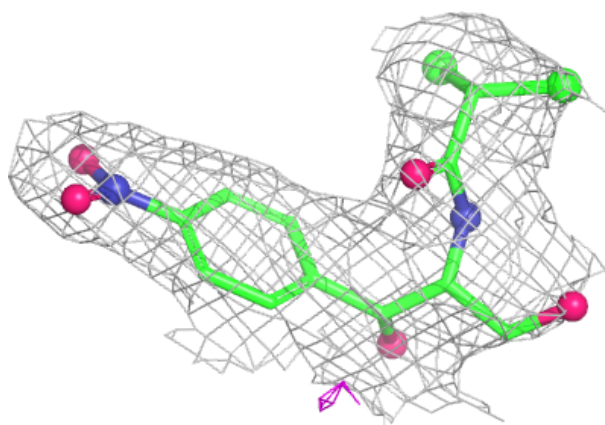
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	3120	1/1	0.99	0.04	44,44,44,44	0
60	MG	BA	3076	1/1	0.99	0.05	31,31,31,31	0
60	MG	AA	1642	1/1	0.99	0.04	42,42,42,42	0
60	MG	BA	3038	1/1	0.99	0.05	21,21,21,21	0
60	MG	BA	3039	1/1	0.99	0.12	9,9,9,9	0
60	MG	BA	3126	1/1	0.99	0.04	32,32,32,32	0
60	MG	BA	3048	1/1	1.00	0.02	18,18,18,18	0
60	MG	BA	3071	1/1	1.00	0.03	8,8,8,8	0
60	MG	BA	3023	1/1	1.00	0.04	8,8,8,8	0
60	MG	BA	3128	1/1	1.00	0.02	6,6,6,6	0
60	MG	BA	3129	1/1	1.00	0.07	15,15,15,15	0
60	MG	BA	3012	1/1	1.00	0.03	5,5,5,5	0
60	MG	BA	3099	1/1	1.00	0.04	32,32,32,32	0
60	MG	BA	3074	1/1	1.00	0.08	15,15,15,15	0
60	MG	BA	3133	1/1	1.00	0.04	5,5,5,5	0
60	MG	BA	3016	1/1	1.00	0.03	5,5,5,5	0
60	MG	BA	3102	1/1	1.00	0.04	14,14,14,14	0
60	MG	BA	3036	1/1	1.00	0.04	30,30,30,30	0
60	MG	BA	3053	1/1	1.00	0.02	35,35,35,35	0
60	MG	BA	3105	1/1	1.00	0.06	11,11,11,11	0
60	MG	BA	3037	1/1	1.00	0.04	7,7,7,7	0
60	MG	BA	3013	1/1	1.00	0.07	6,6,6,6	0
60	MG	BA	3018	1/1	1.00	0.17	10,10,10,10	0
60	MG	BA	3040	1/1	1.00	0.03	11,11,11,11	0
60	MG	BA	3041	1/1	1.00	0.03	12,12,12,12	0
60	MG	BA	3019	1/1	1.00	0.08	50,50,50,50	0
60	MG	BA	3084	1/1	1.00	0.02	9,9,9,9	0
60	MG	BA	3043	1/1	1.00	0.13	19,19,19,19	0
60	MG	BA	3020	1/1	1.00	0.03	21,21,21,21	0
60	MG	BA	3062	1/1	1.00	0.03	9,9,9,9	0
60	MG	BA	3116	1/1	1.00	0.04	14,14,14,14	0
60	MG	BA	3063	1/1	1.00	0.01	11,11,11,11	0
60	MG	BA	3064	1/1	1.00	0.02	8,8,8,8	0
60	MG	BA	3065	1/1	1.00	0.03	27,27,27,27	0
60	MG	BA	3066	1/1	1.00	0.02	14,14,14,14	0
60	MG	BA	3121	1/1	1.00	0.02	5,5,5,5	0
60	MG	BA	3021	1/1	1.00	0.02	15,15,15,15	0
60	MG	AA	1641	1/1	1.00	0.05	27,27,27,27	0
60	MG	BA	3032	1/1	1.00	0.04	6,6,6,6	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.

Electron density around CLM BA 3136:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.